

Supporting Information

Base-mediated 1,3-dipolar cycloaddition of pyridinium bromides with bromoallyl sulfones: A facile access to indolizine scaffolds

Chetna Jadala,^{‡, a} Velma Ganga Reddy,^{‡, b, c} Namballa Hari Krishna,^{a, b, d} Nagula Shankaraiah,^{*a} and Ahmed Kamal^{*a, b, e}

^a*Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad 500037, India.*

^b*Medicinal Chemistry and Pharmacology, CSIR-Indian Institute of Chemical Technology, Hyderabad 500007, India.*

^c*Centre for Advanced Materials & Industrial Chemistry (CAMIC), School of Science, RMIT University, GPO Box 2476, Melbourne 3001, Australia*

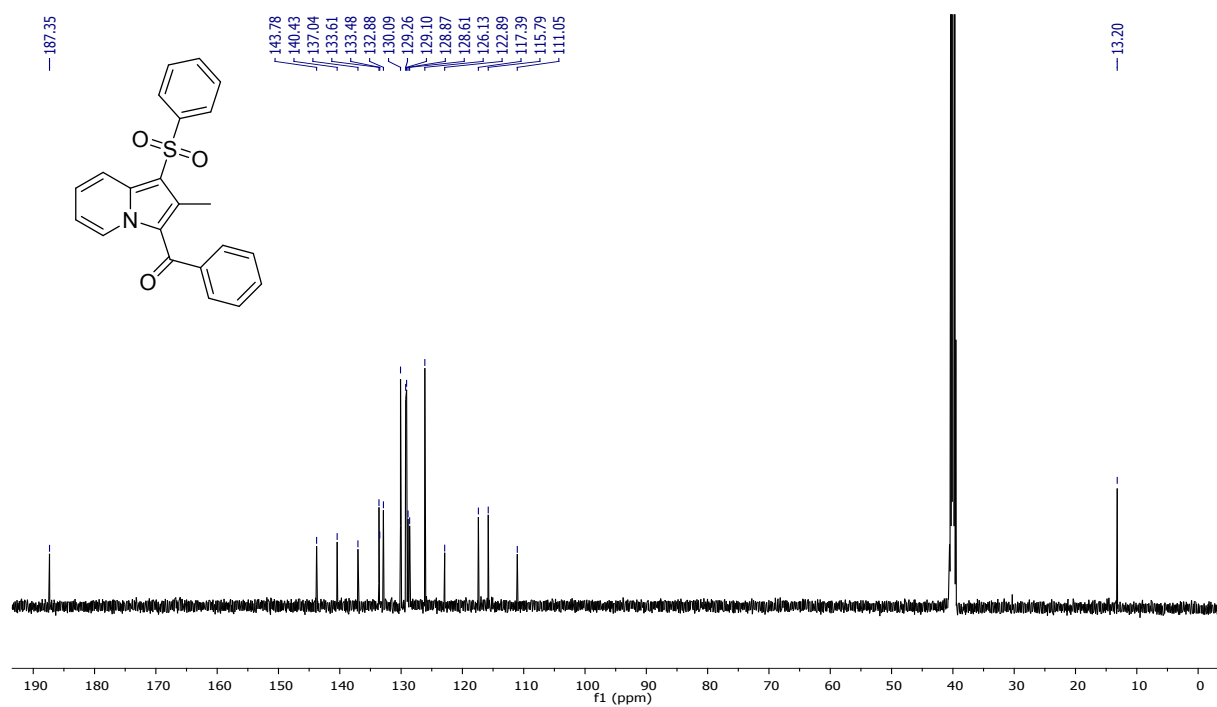
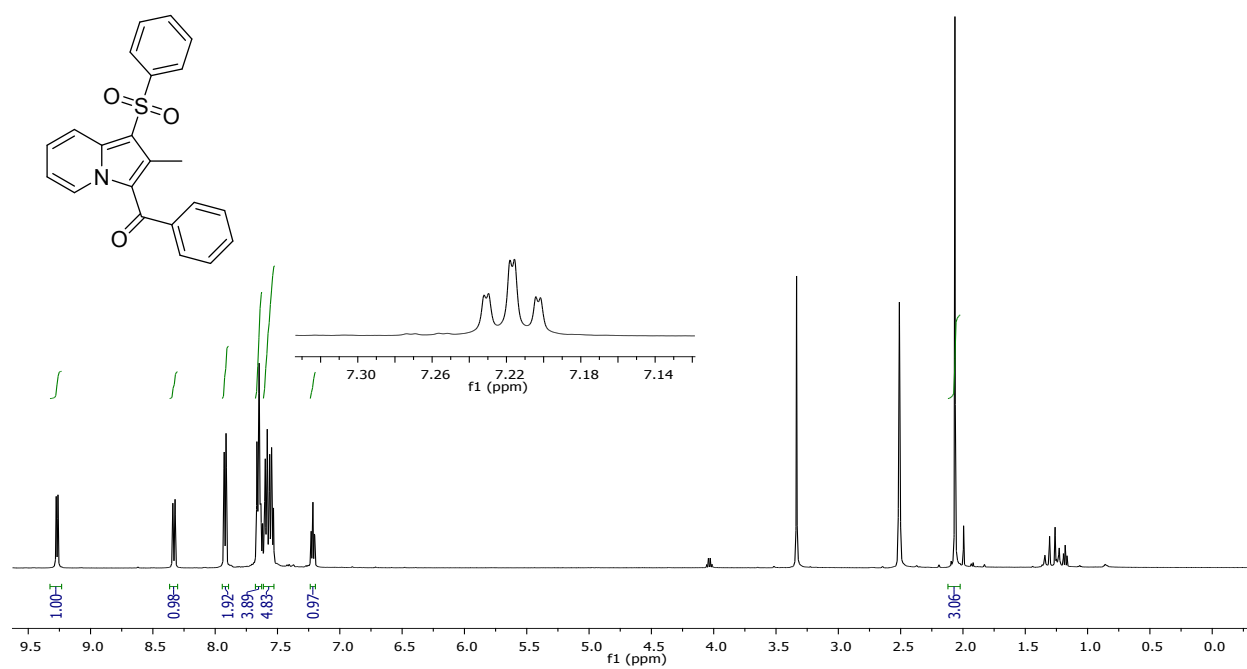
^d*Department of Chemistry, Hunter College, City University of New York, 695 Park Avenue, NY 10065, USA*

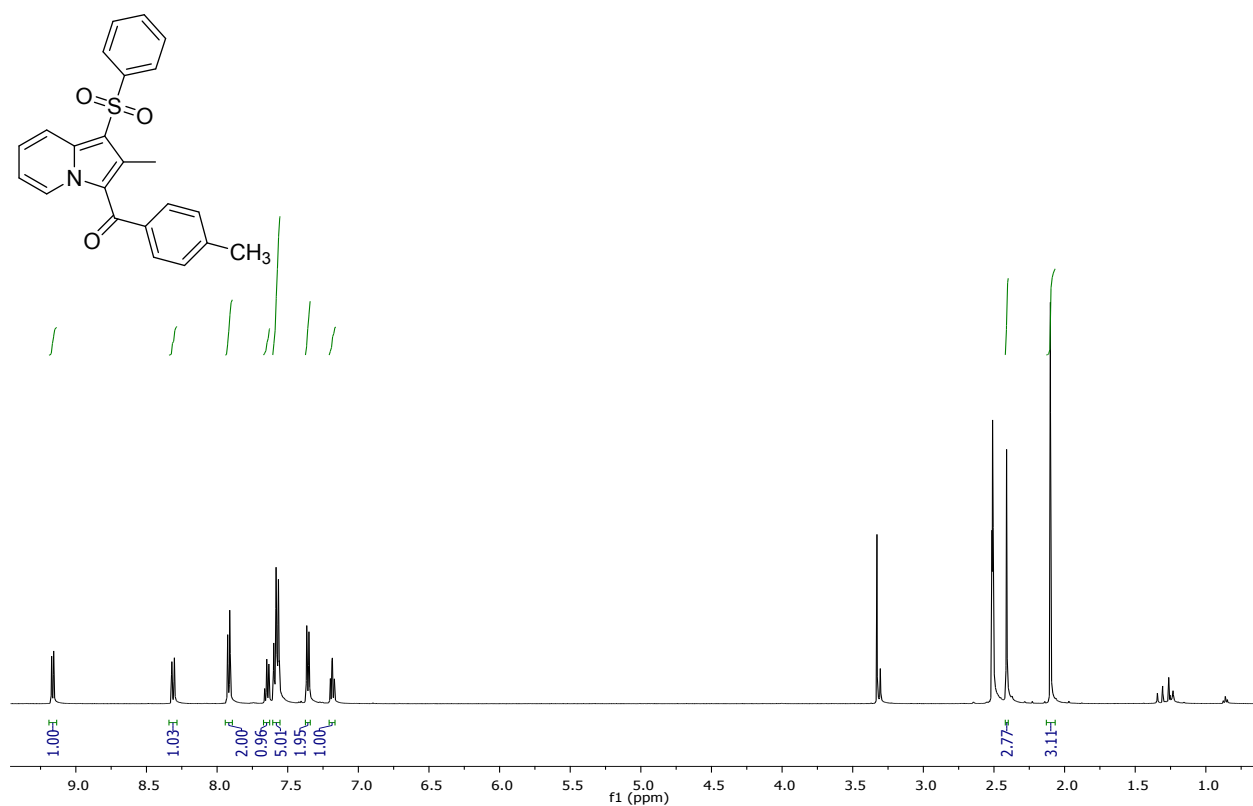
^e*School of Pharmaceutical Education and Research (SPER) Jamia Hamdard, New Delhi, 110062, India.*

[‡] Both the authors share equal authorship

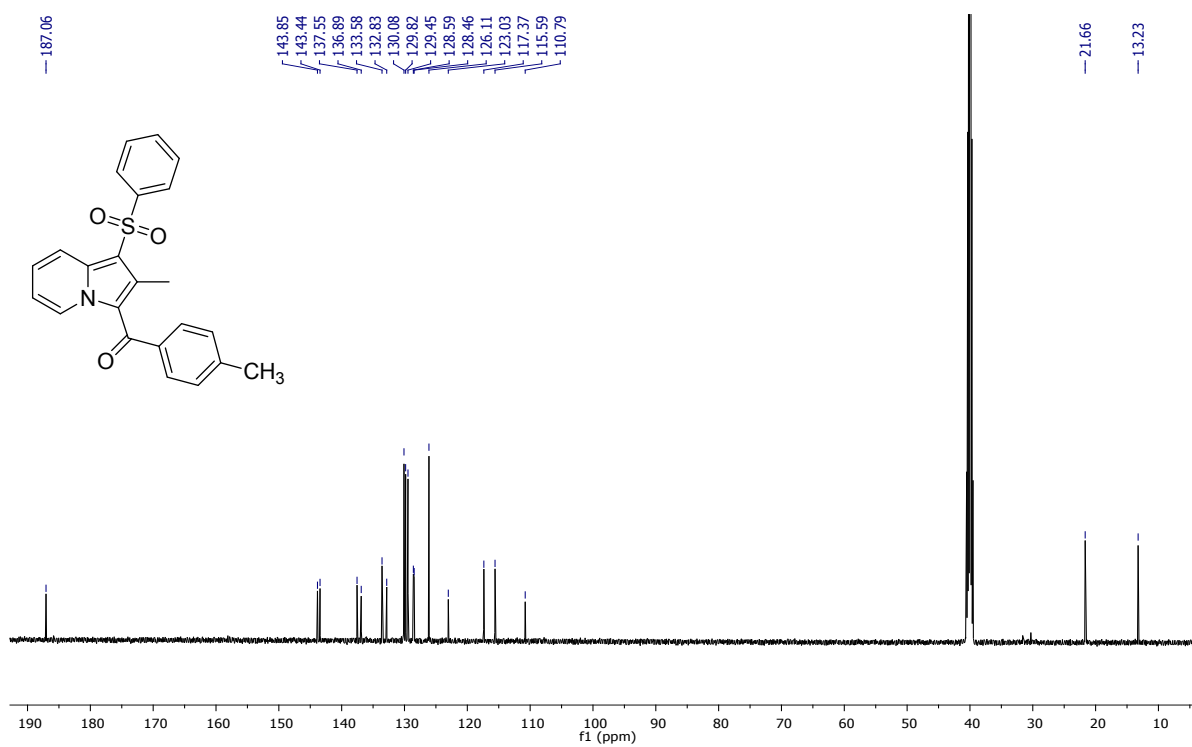
*Corresponding authors: Dr. Ahmed Kamal, E-mail.: ahmedkamal@iict.res.in and Dr. Nagula Shankaraiah, E-mail.: shankar.niperhyd@gov.in

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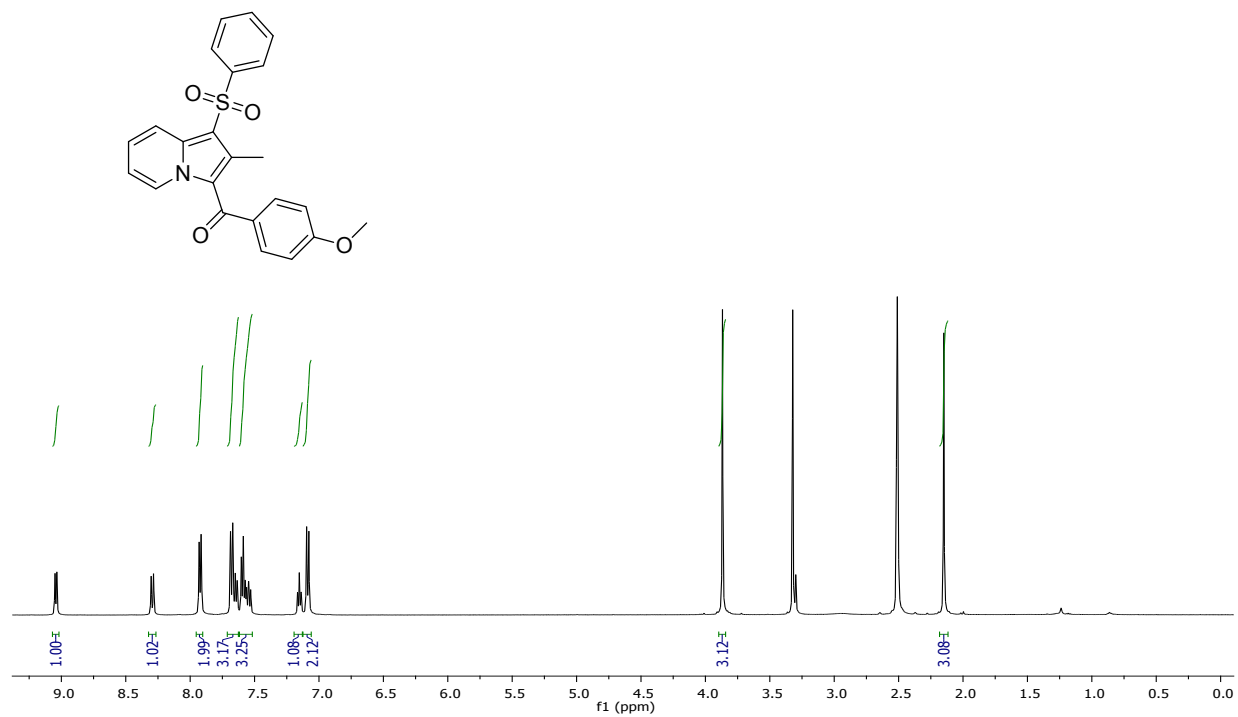




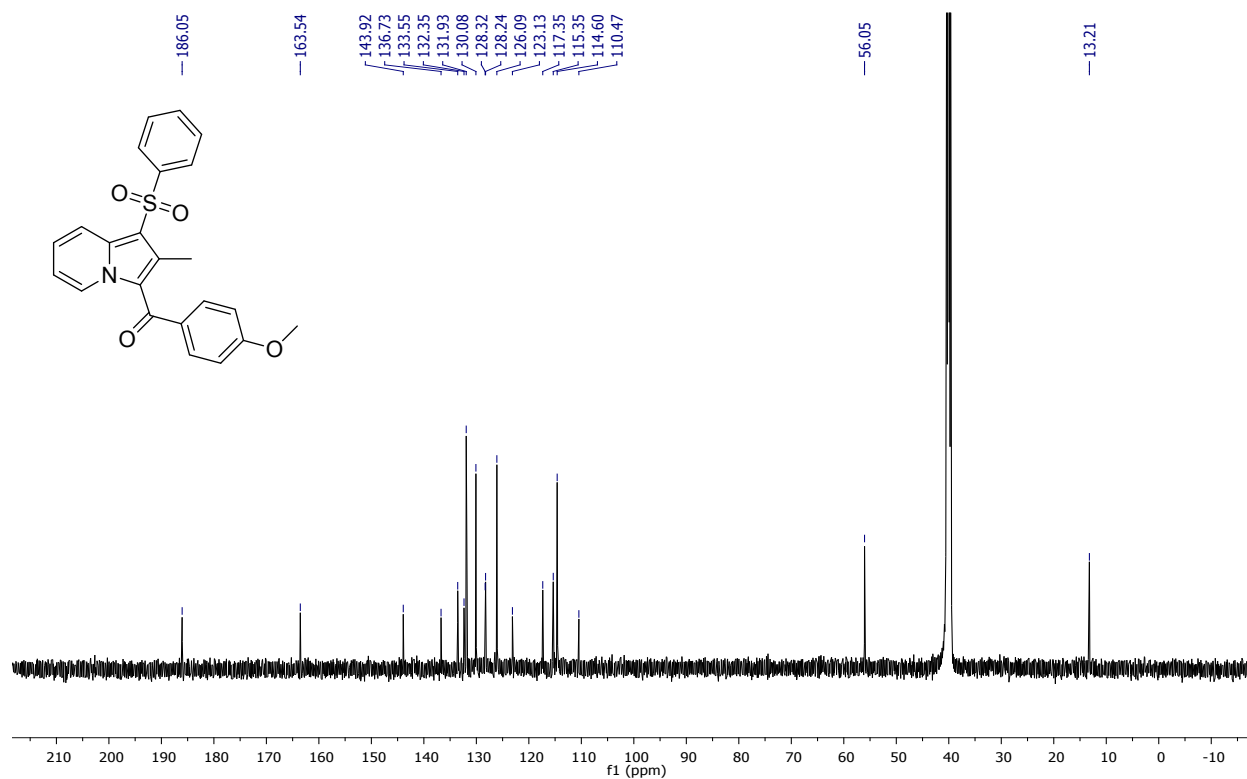
¹H NMR (500 MHz, DMSO-*d*₆) spectrum of **5b**.



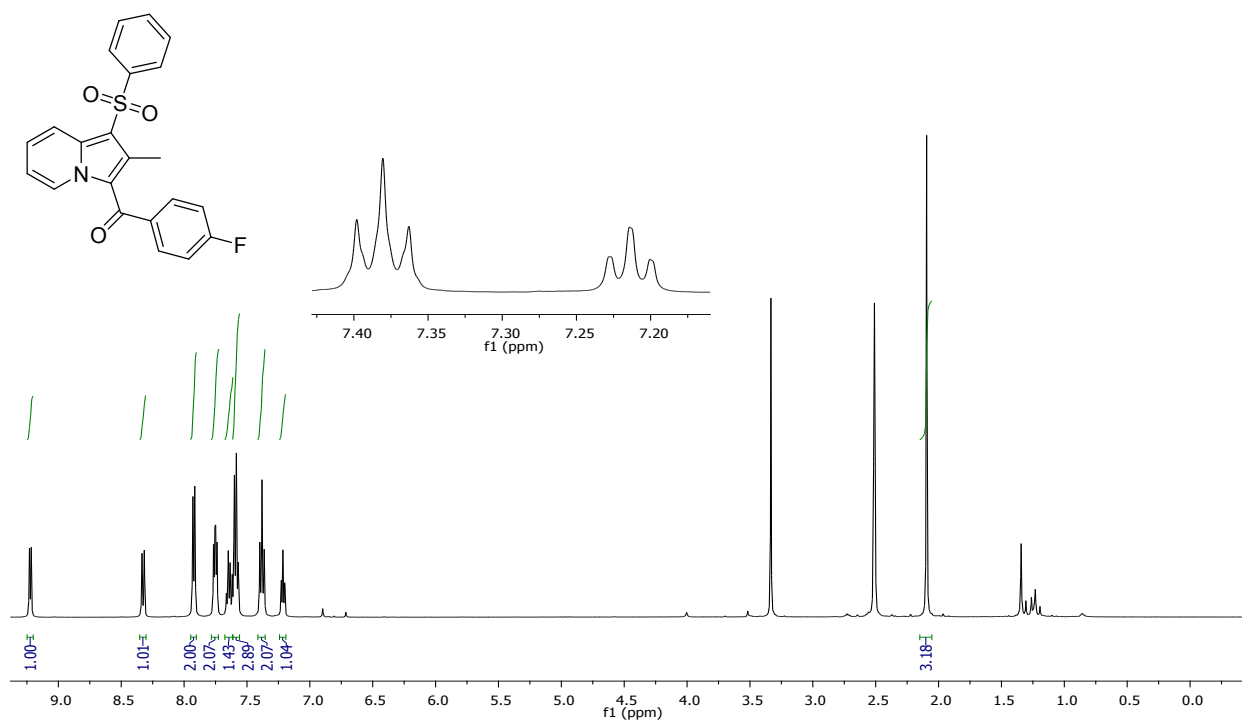
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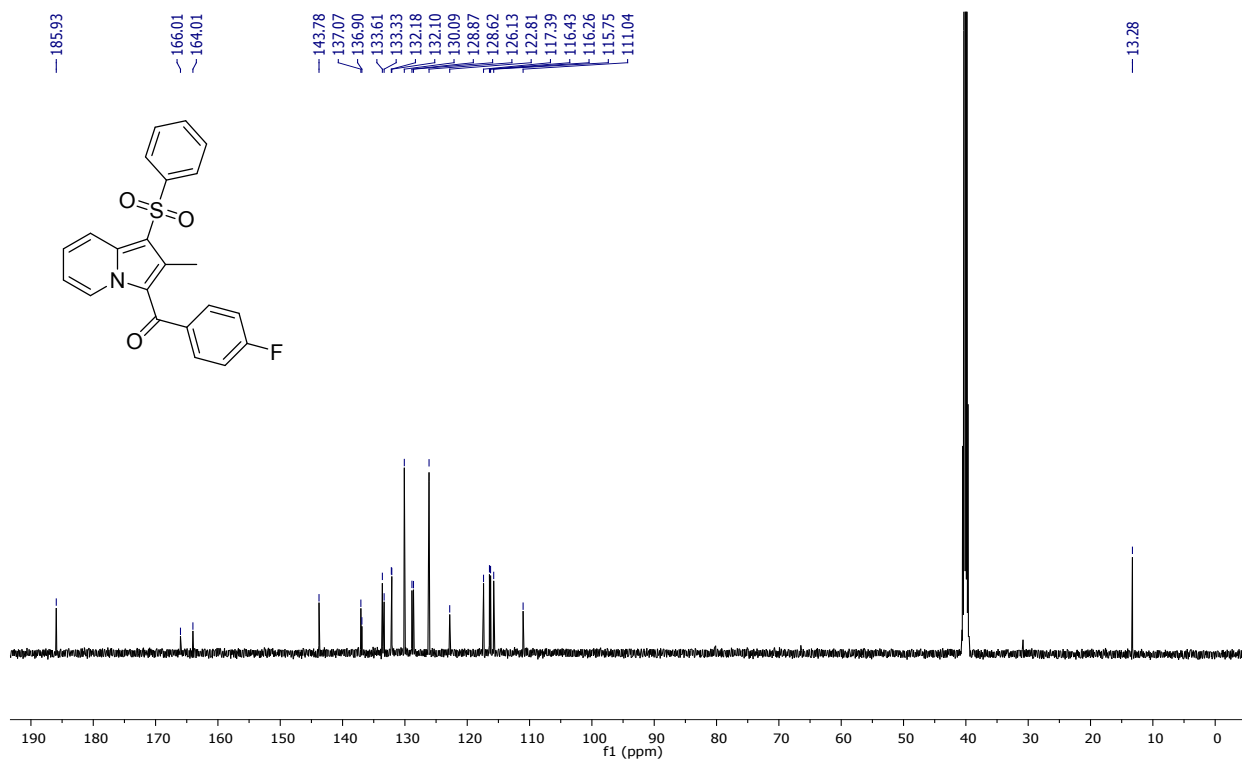
¹H NMR (500 MHz, DMSO-*d*₆) spectrum of **5c**.



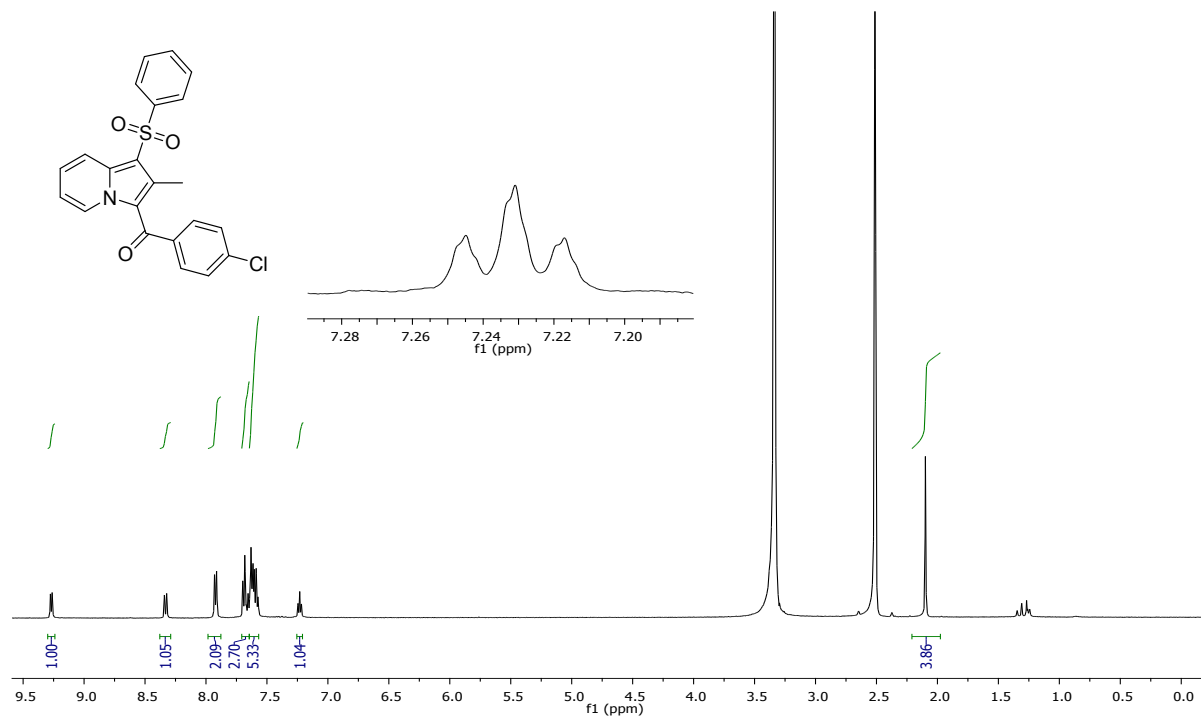
¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of **5c**.



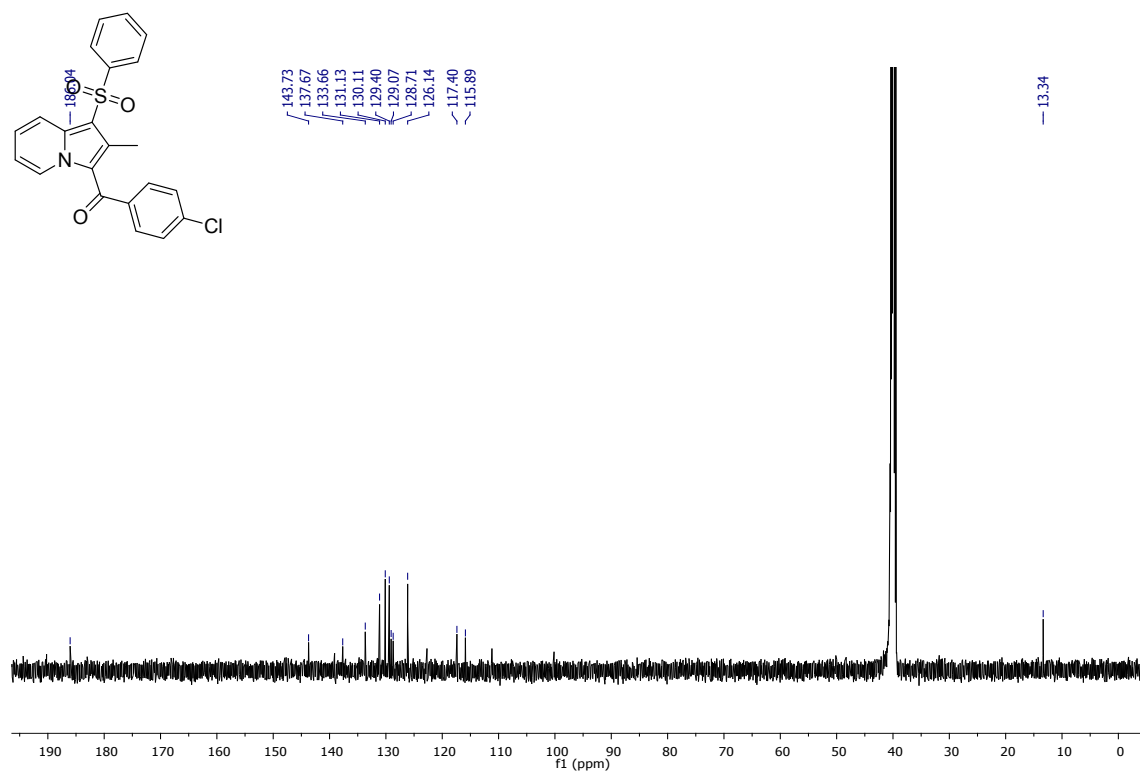
¹H NMR (500 MHz, DMSO-*d*₆) spectrum of **5d**.



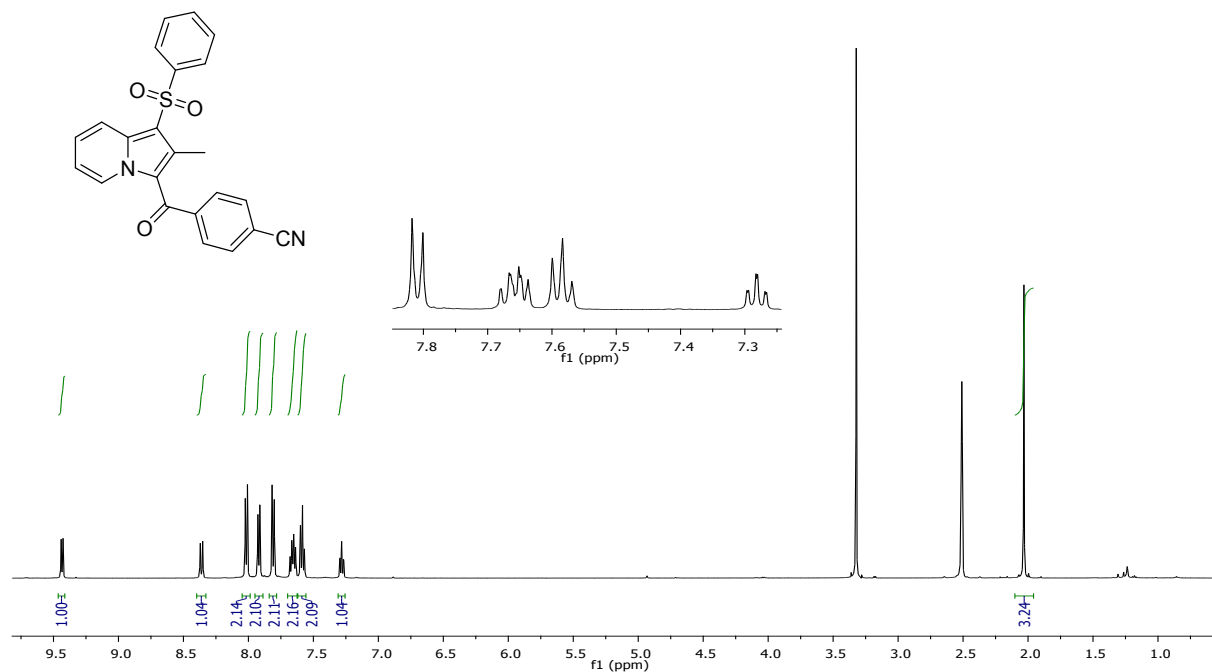
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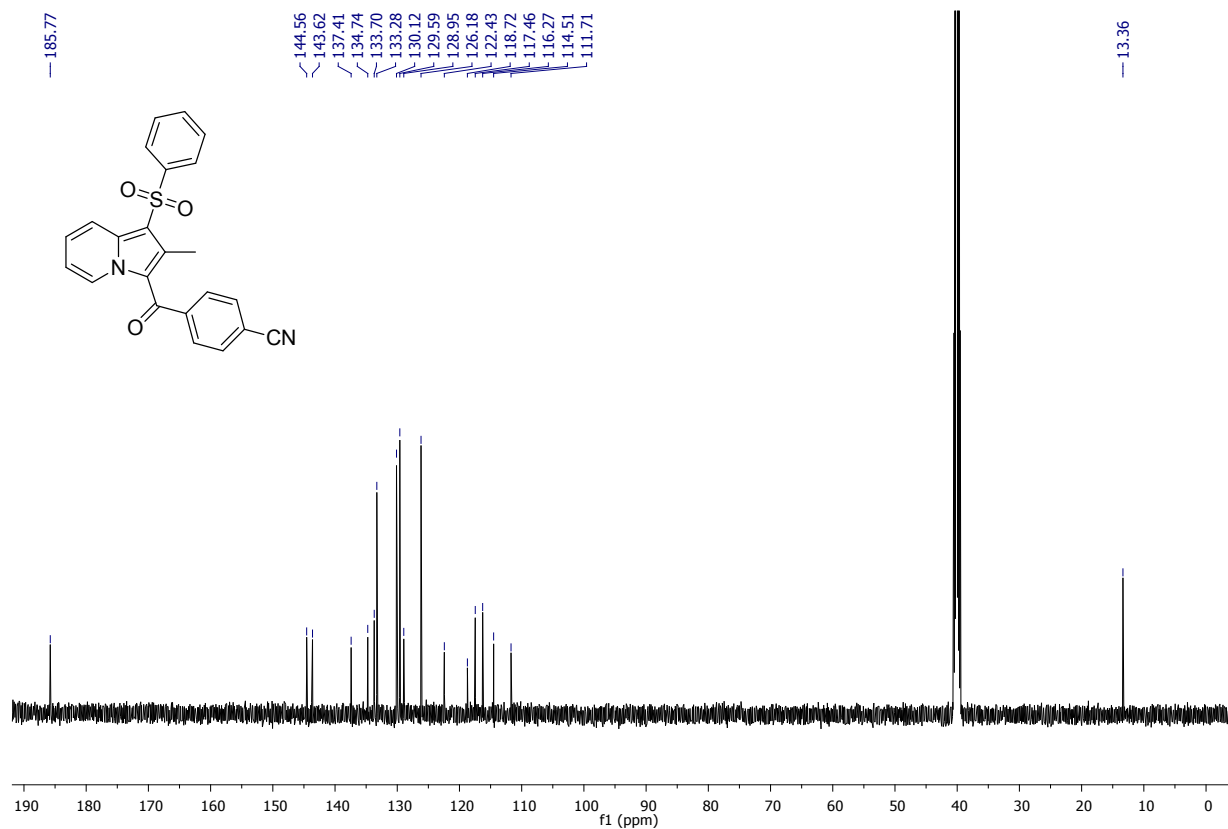
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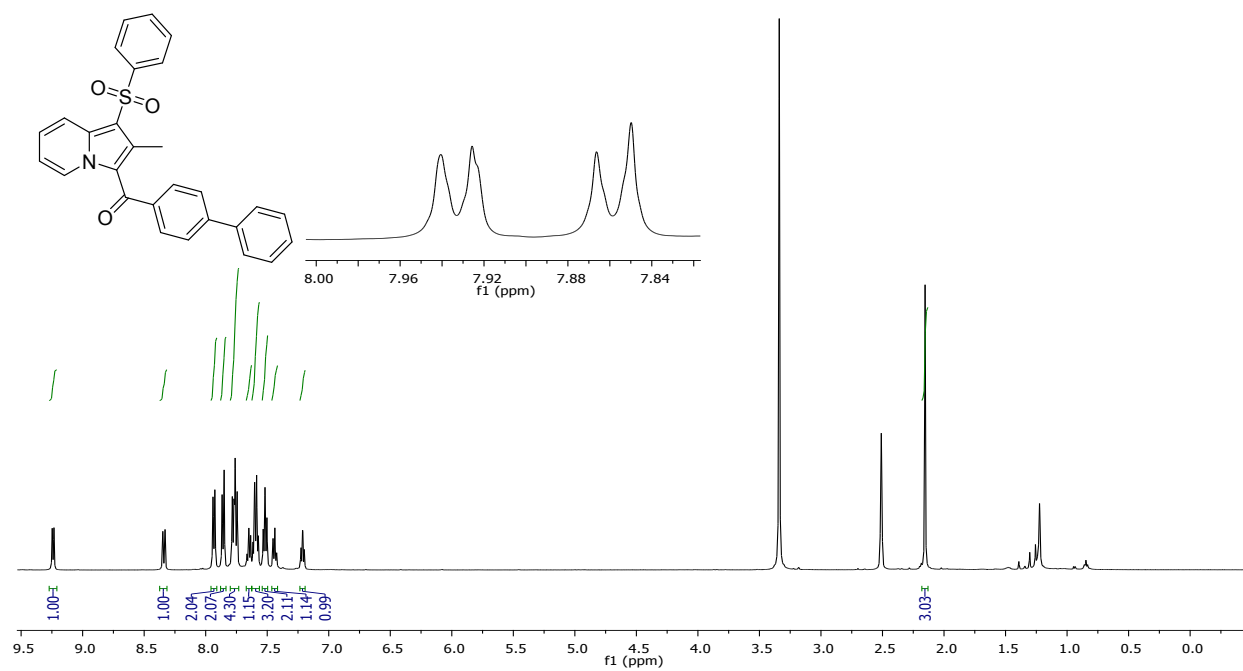
¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of **5e**.



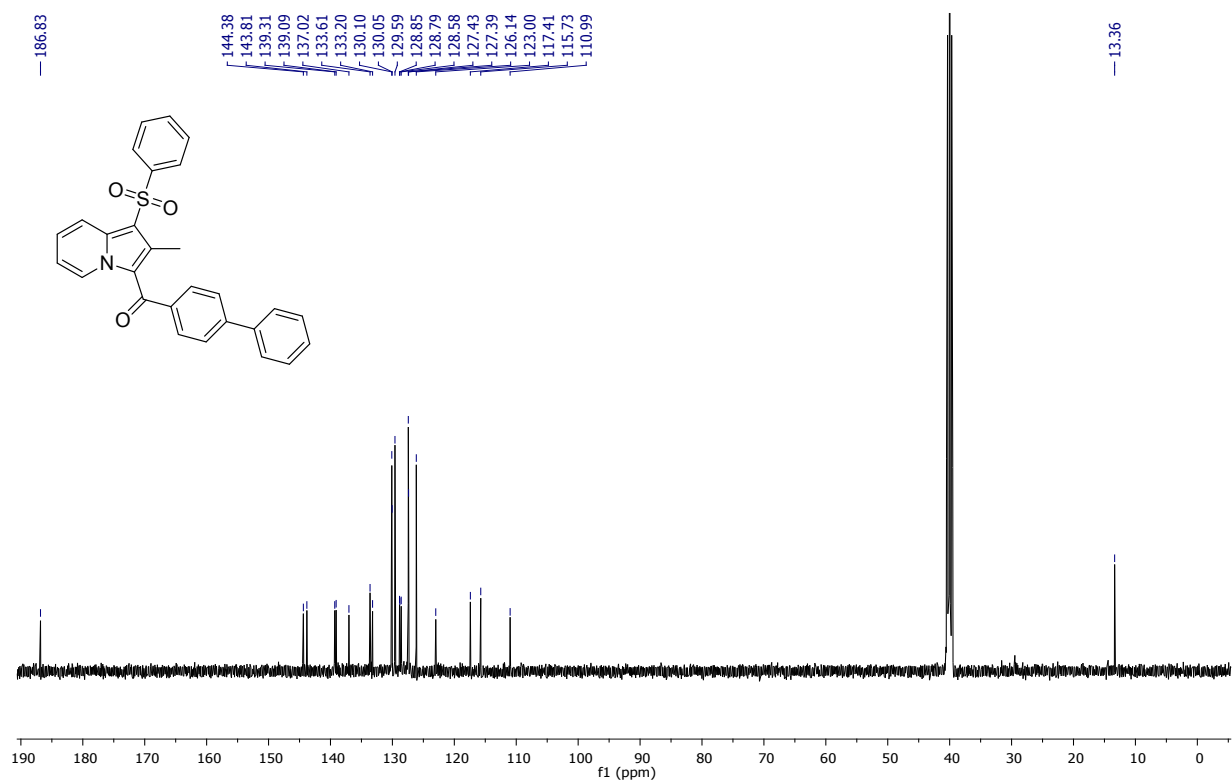
¹H NMR (500 MHz, DMSO-*d*₆) spectrum of **5f**.



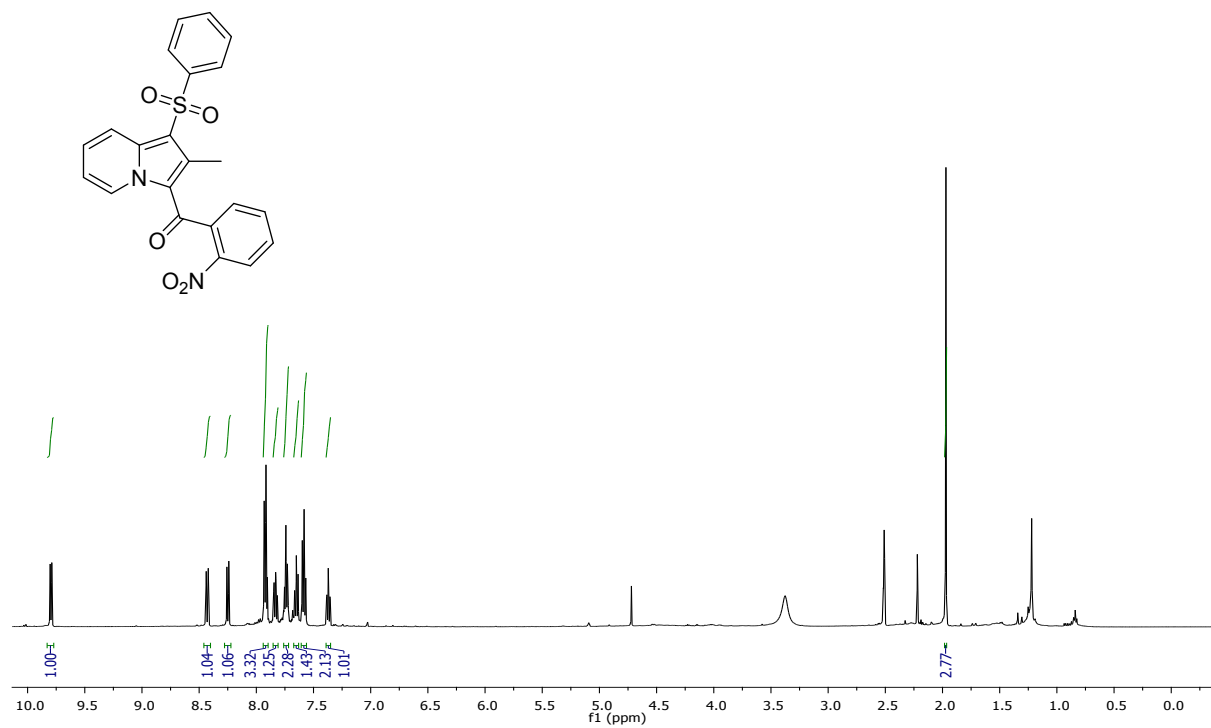
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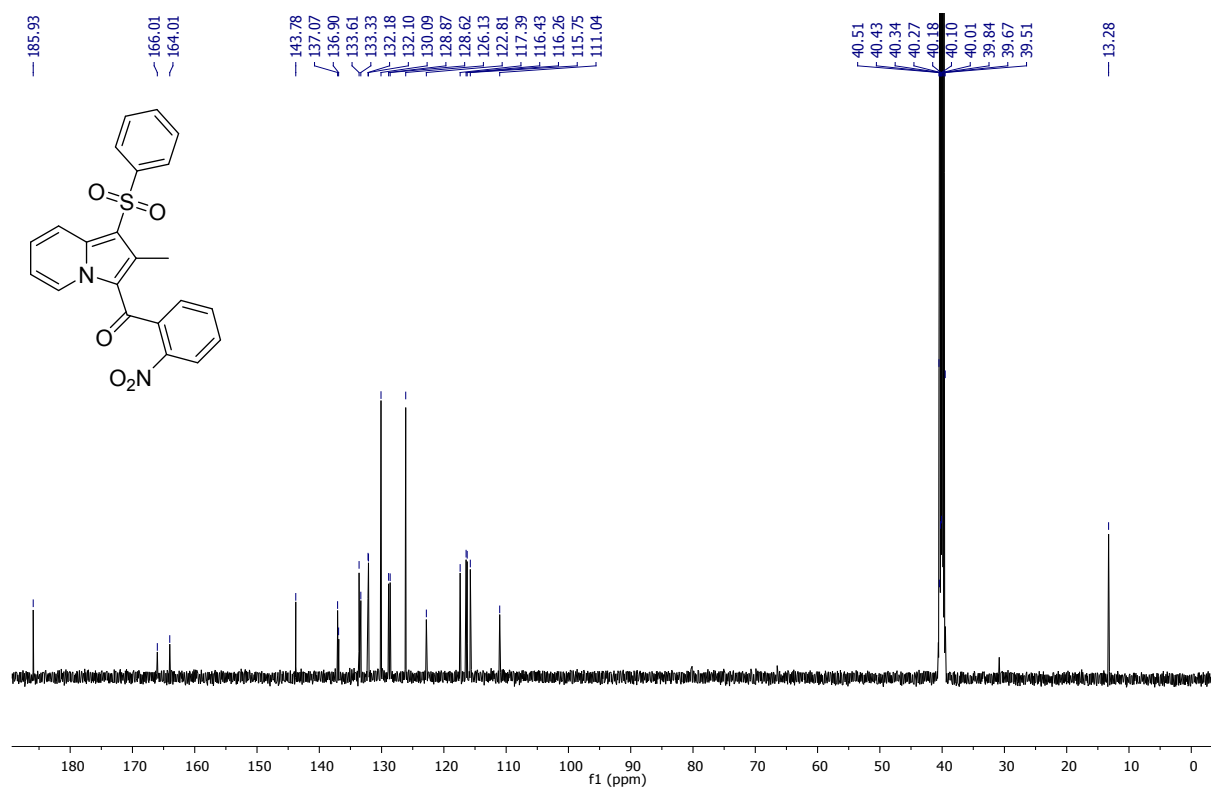
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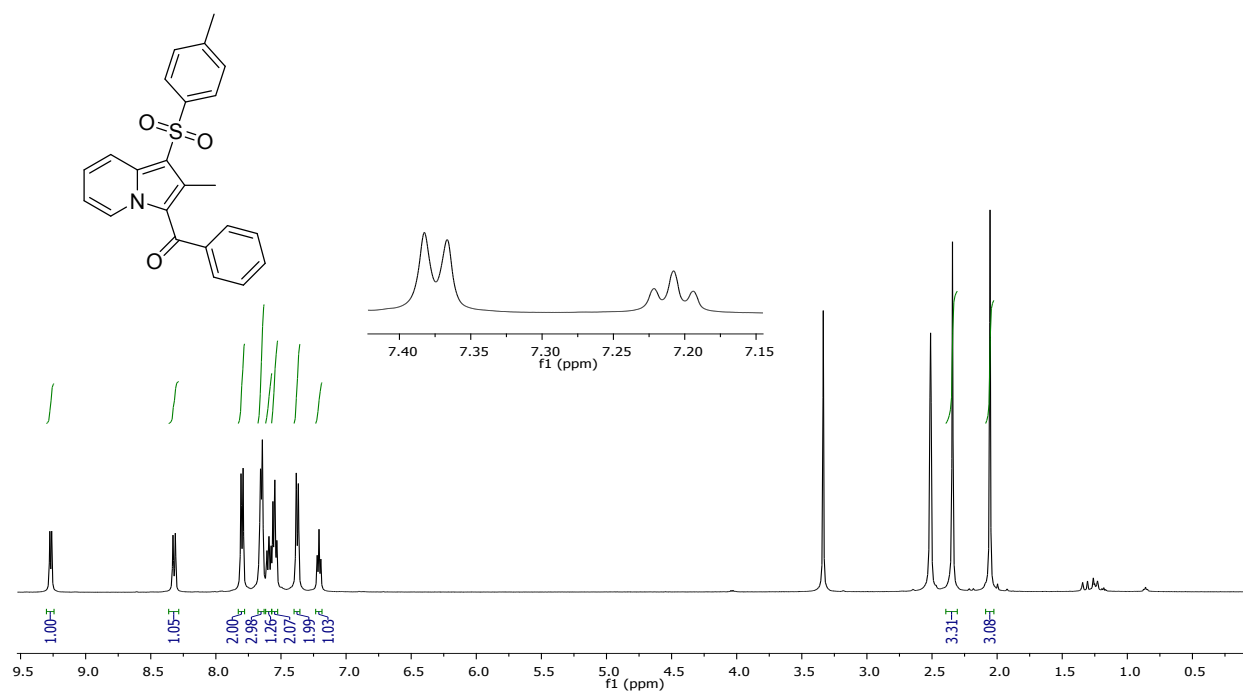
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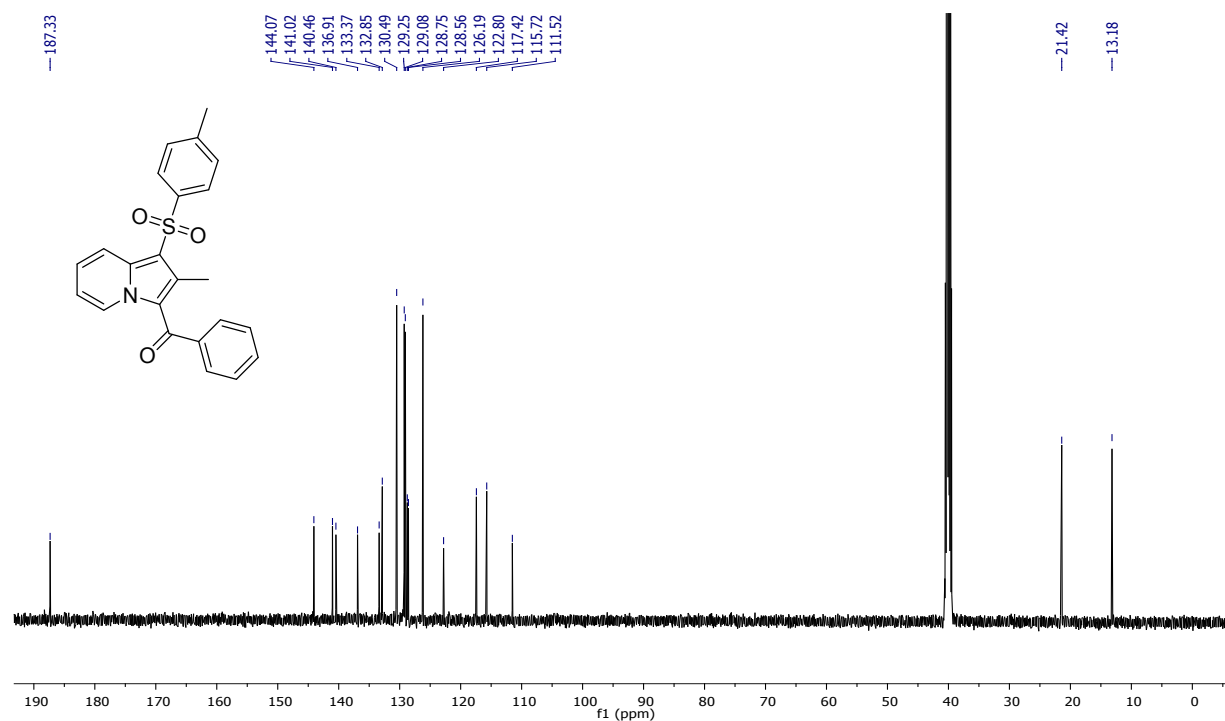
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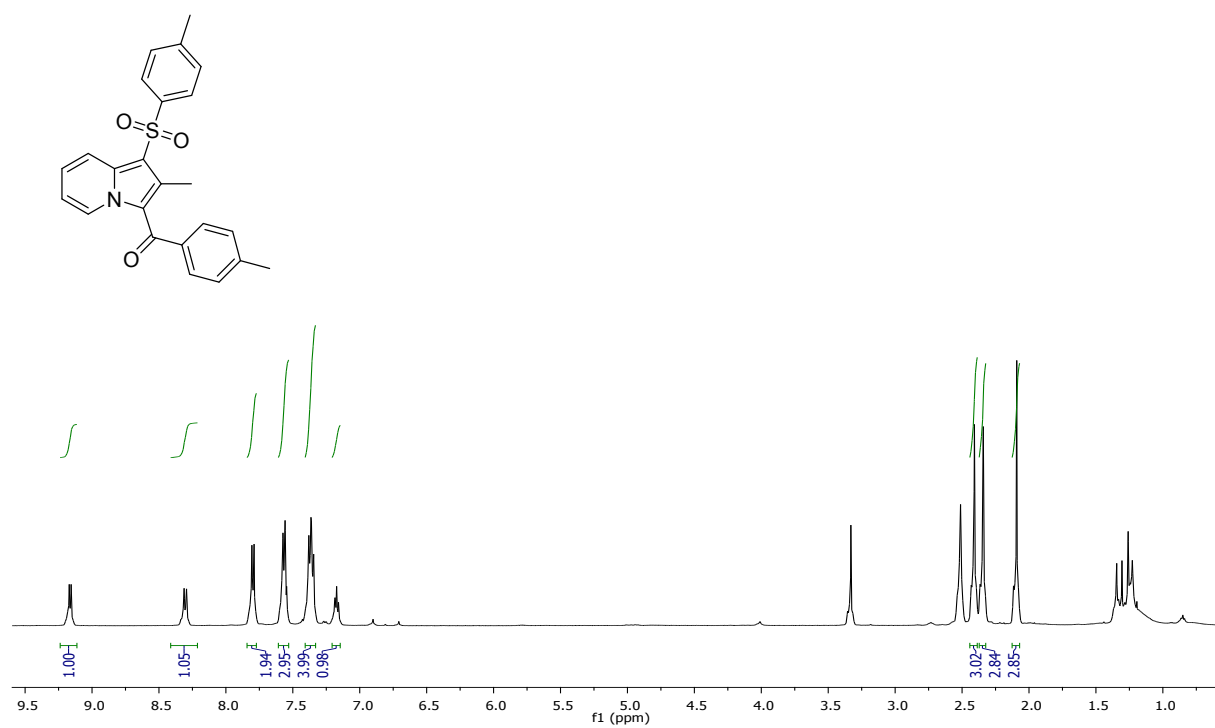
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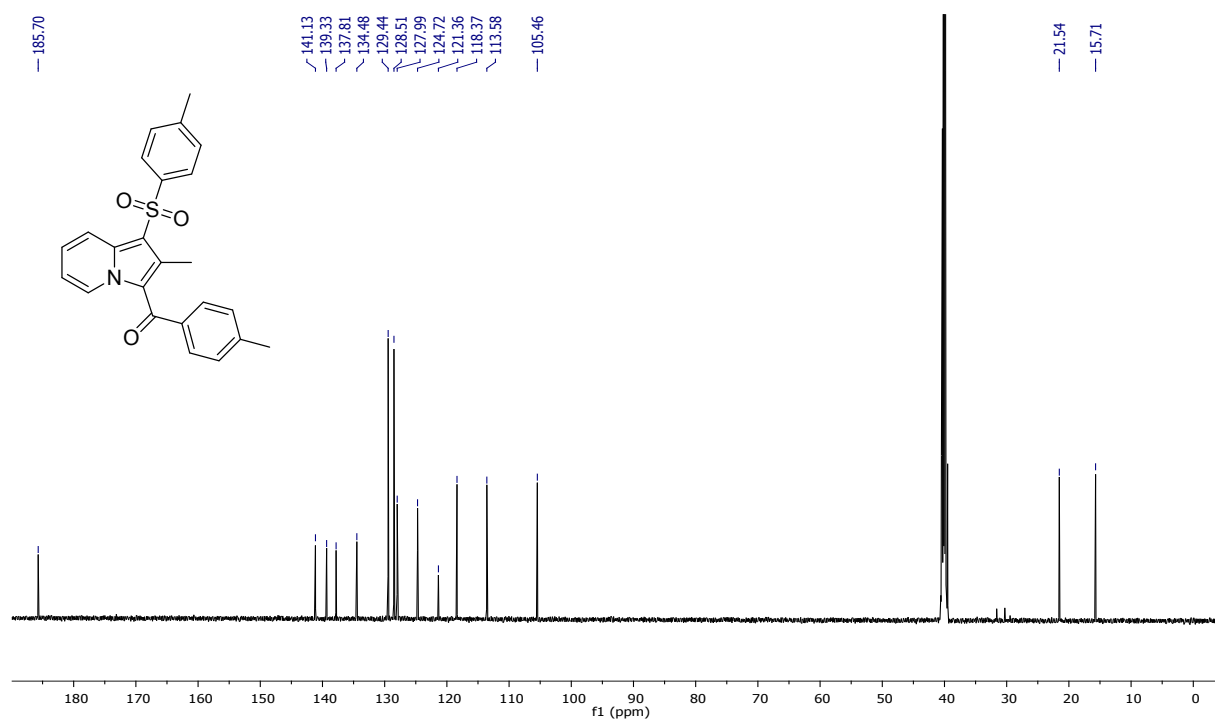
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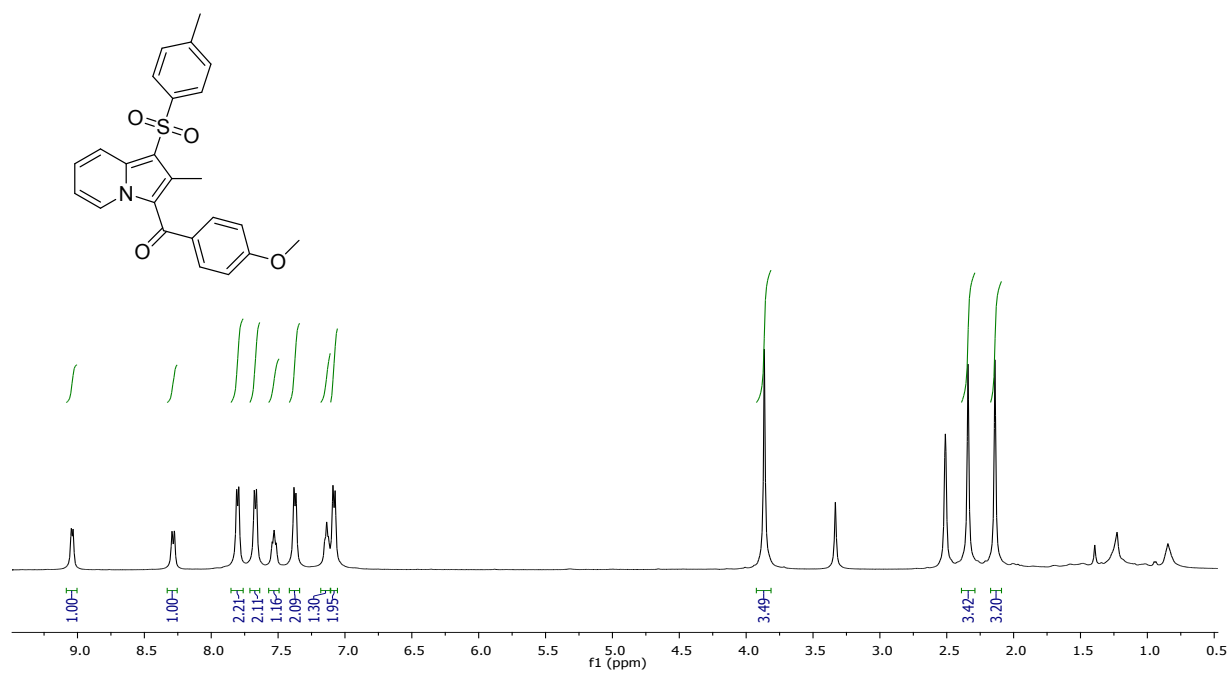
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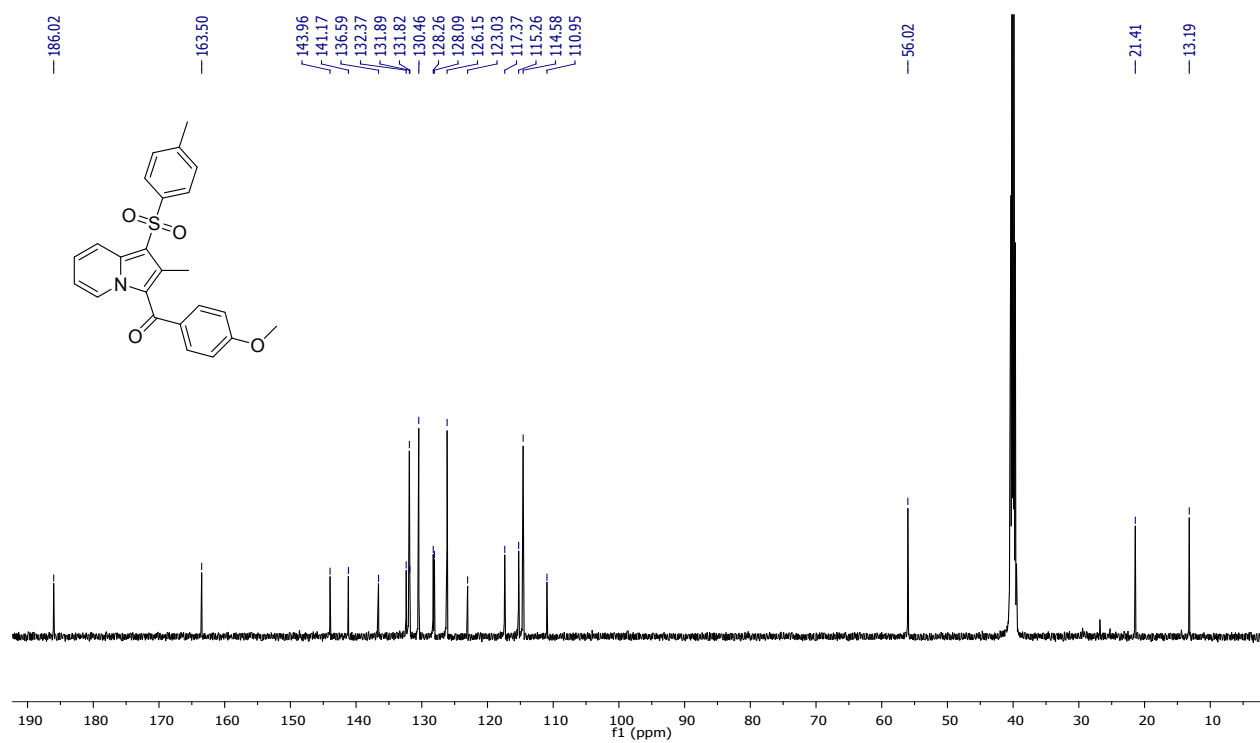
¹H NMR (500 MHz, DMSO-*d*₆) spectrum of **6b**.



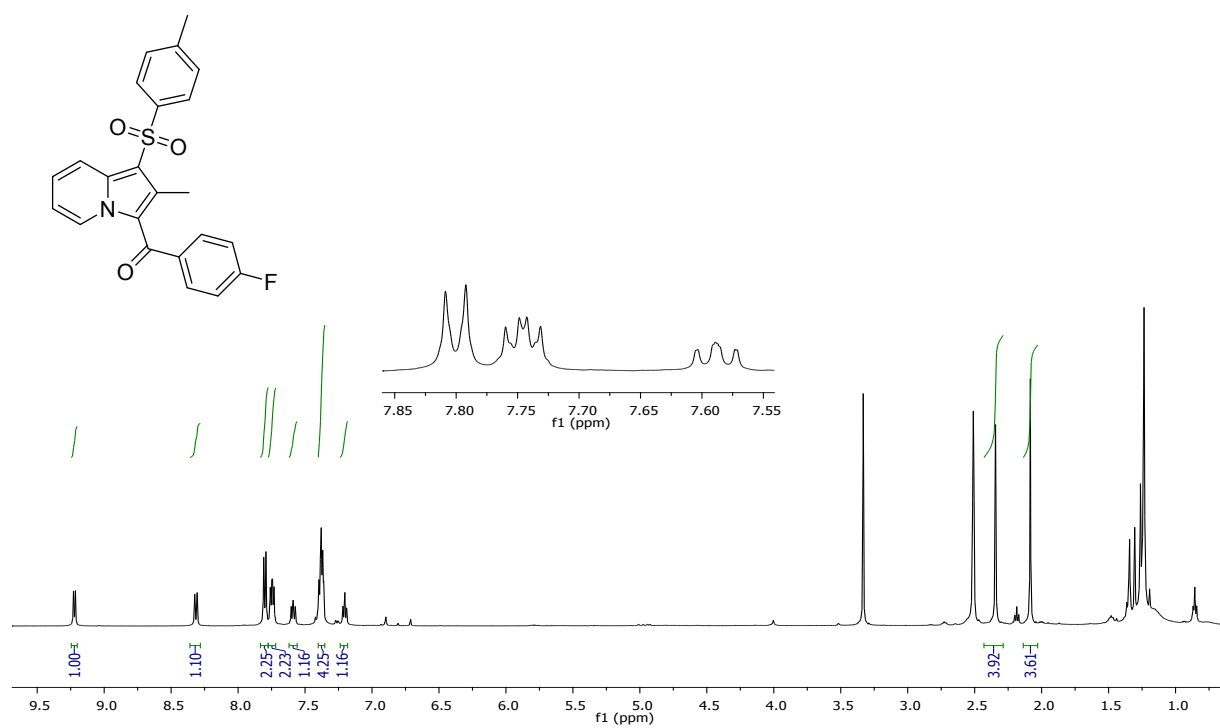
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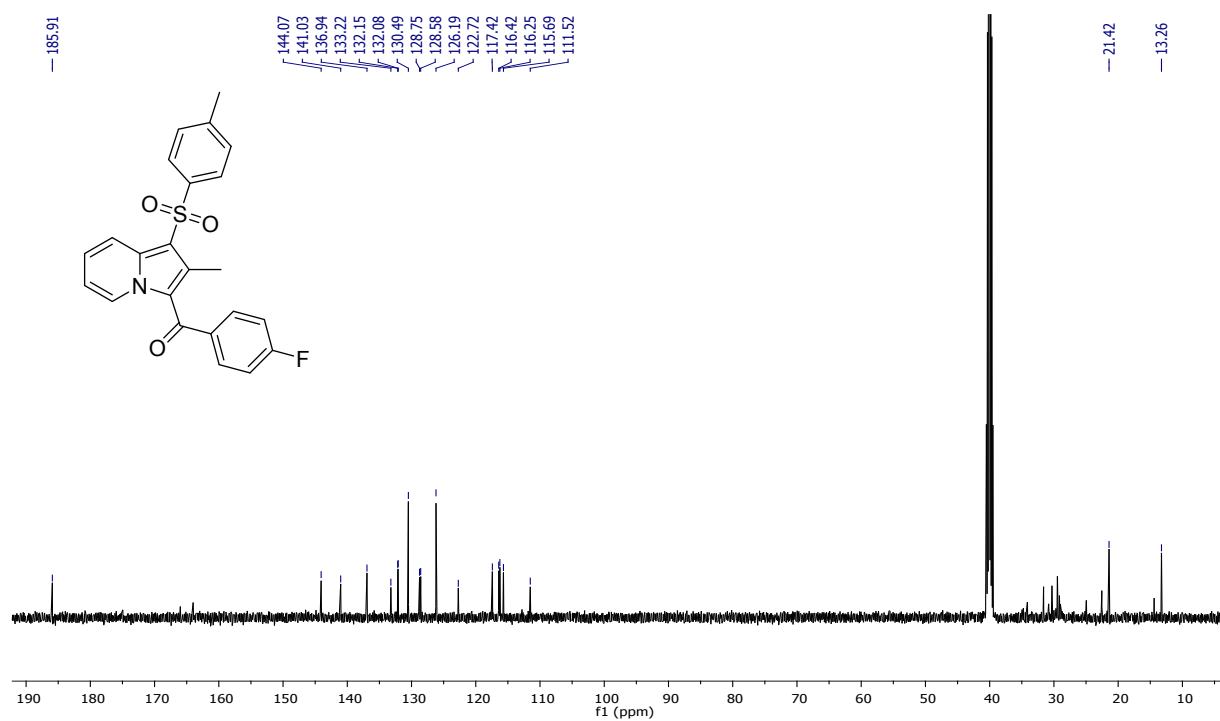
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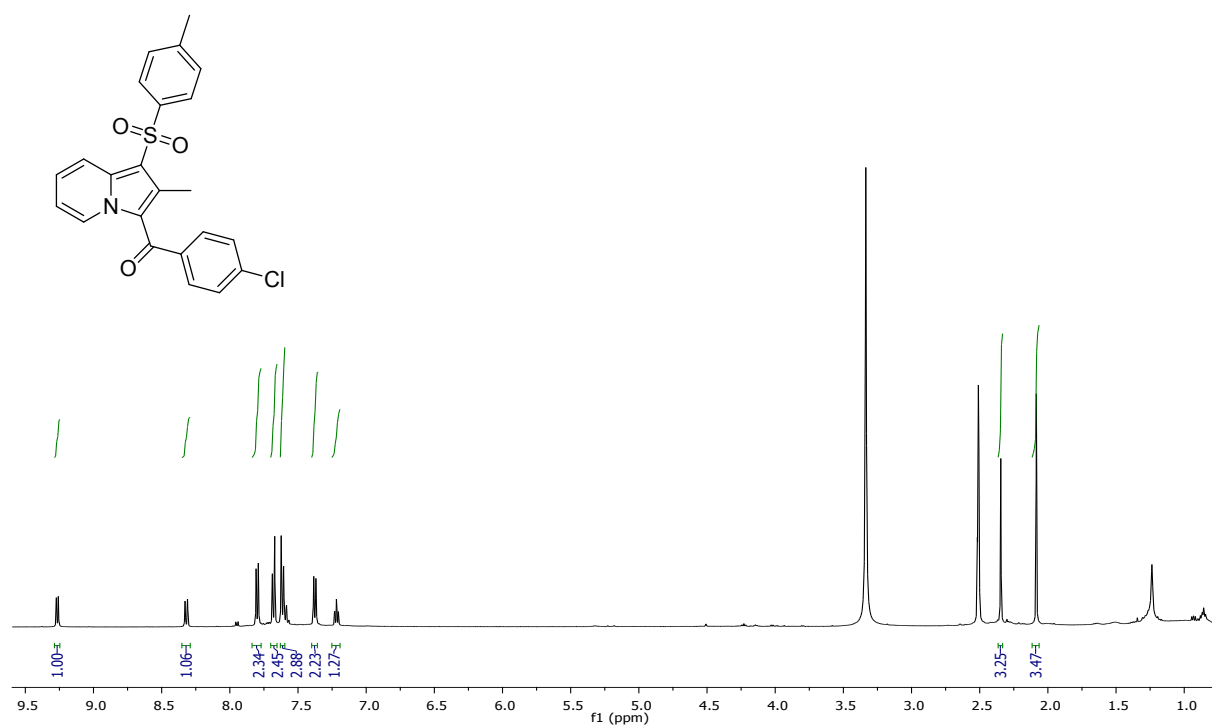
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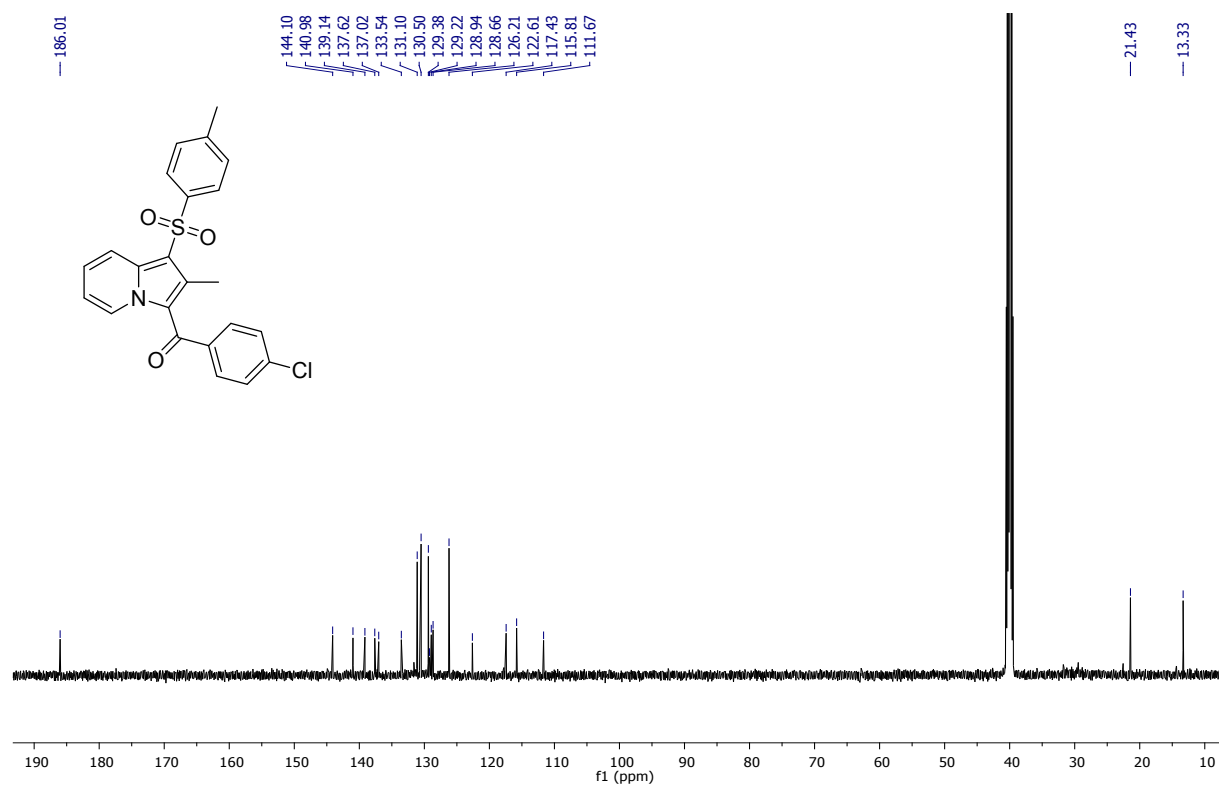
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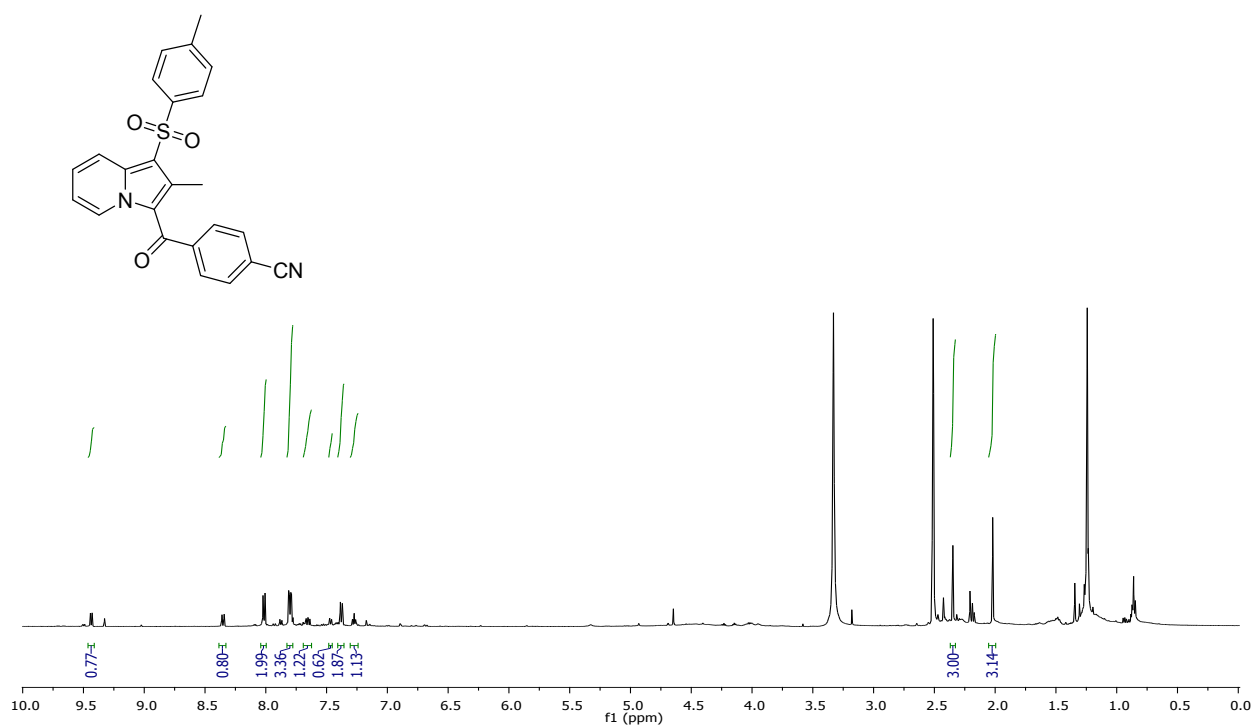
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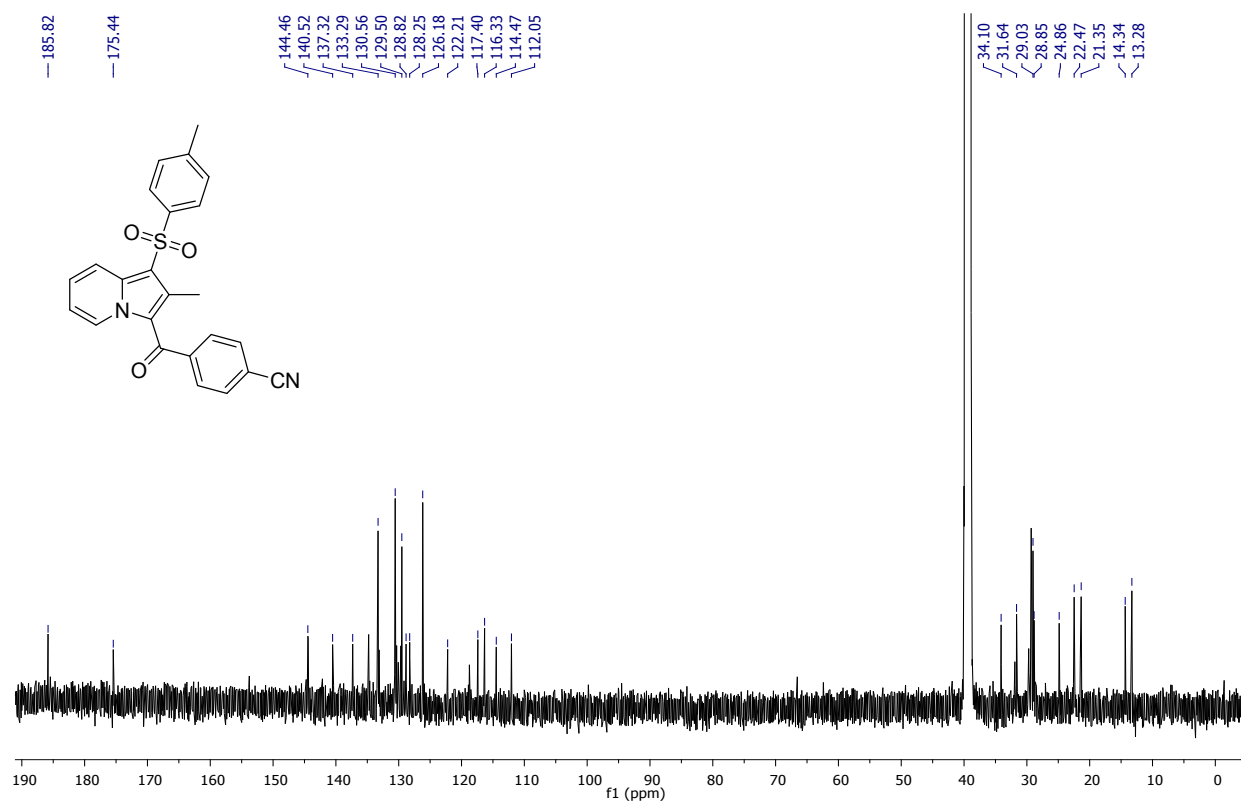
^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of **6e**.



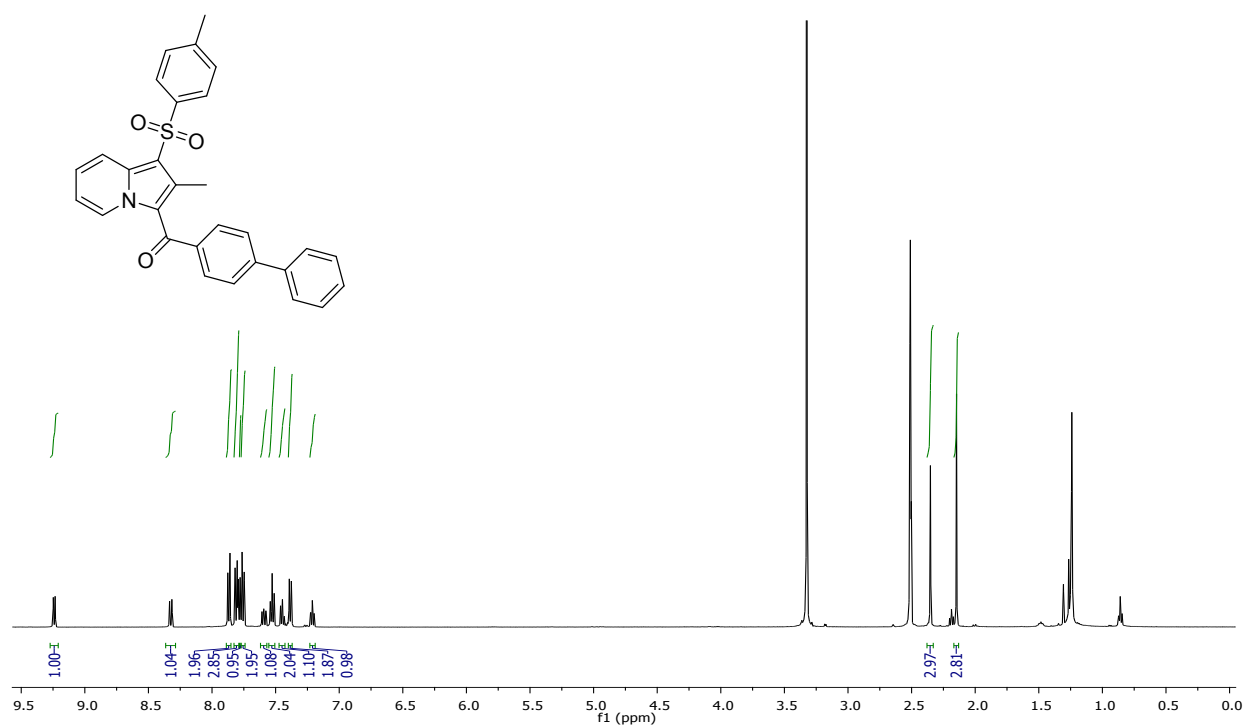
^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) spectrum of **6e**.



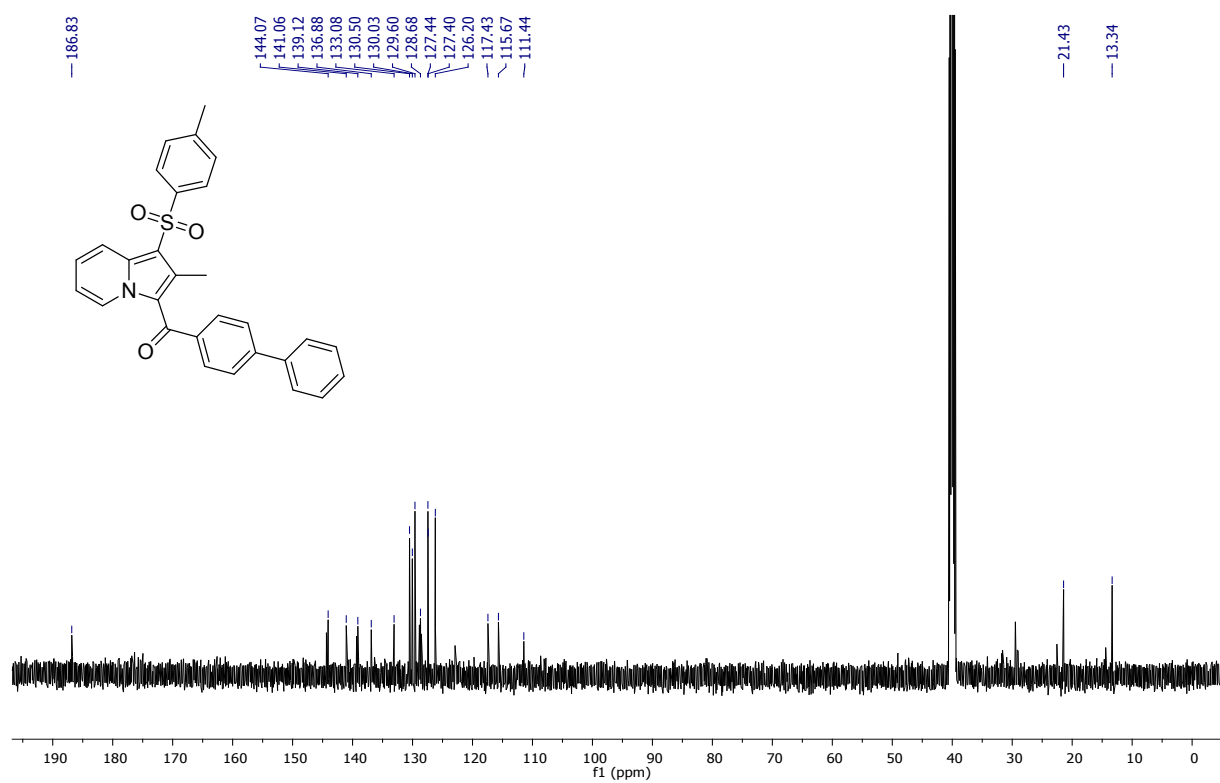
^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of **6f**.



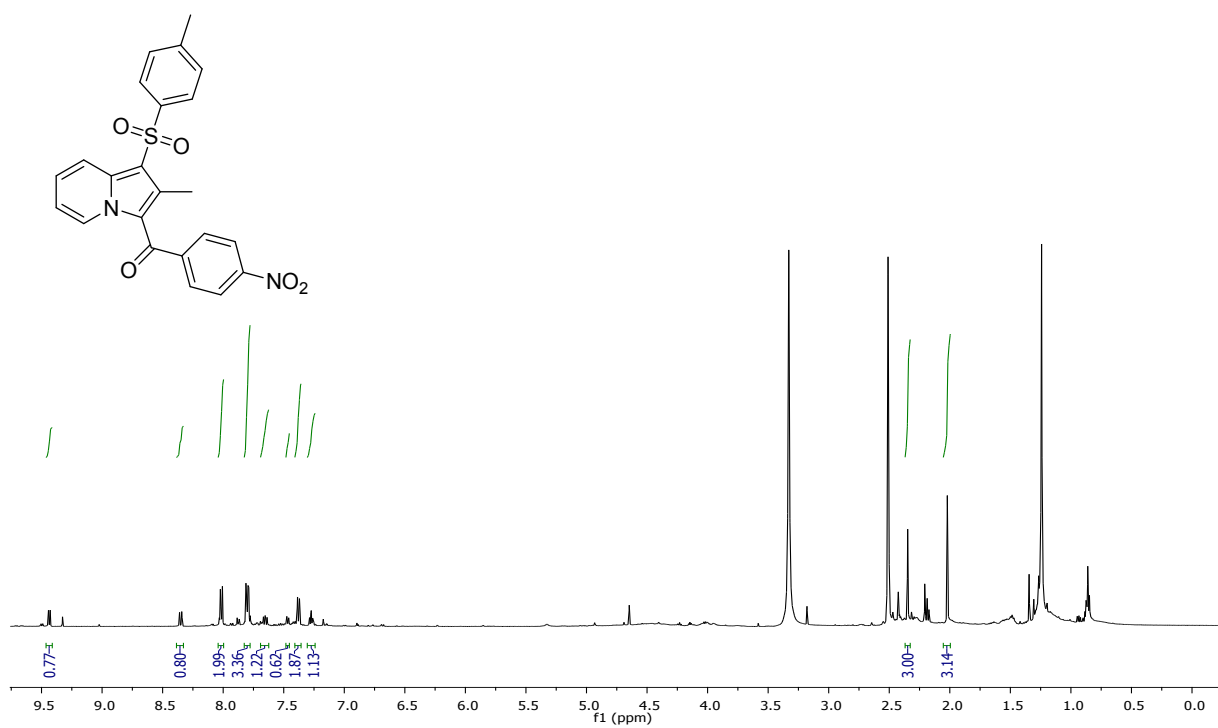
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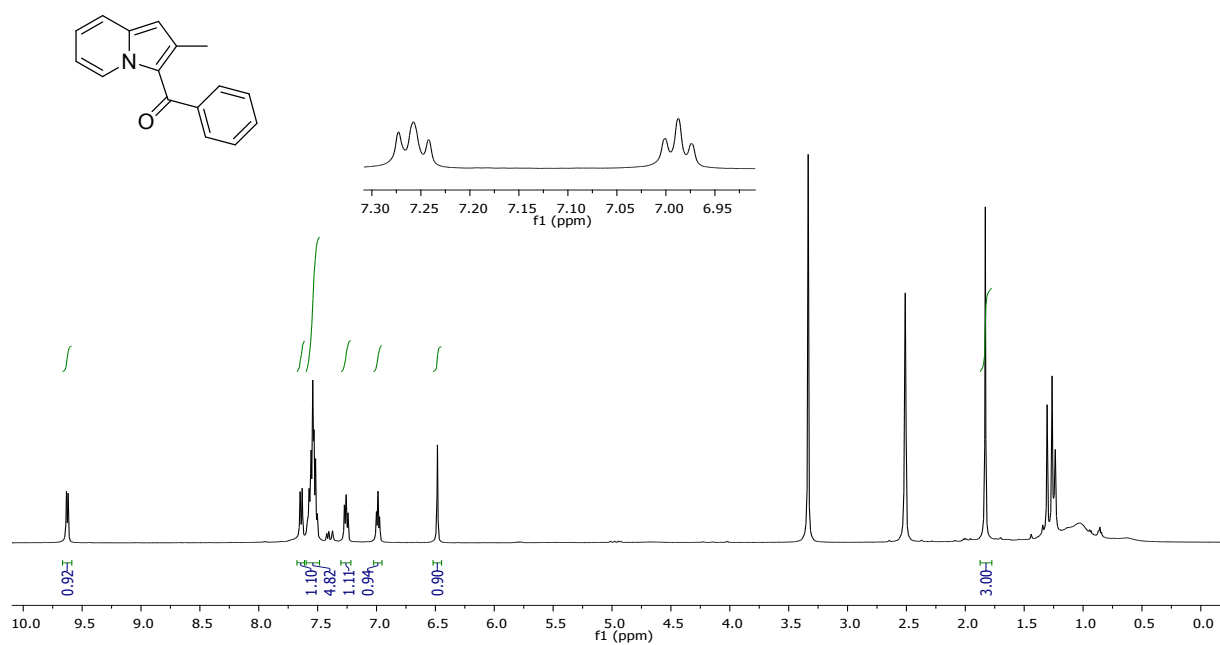
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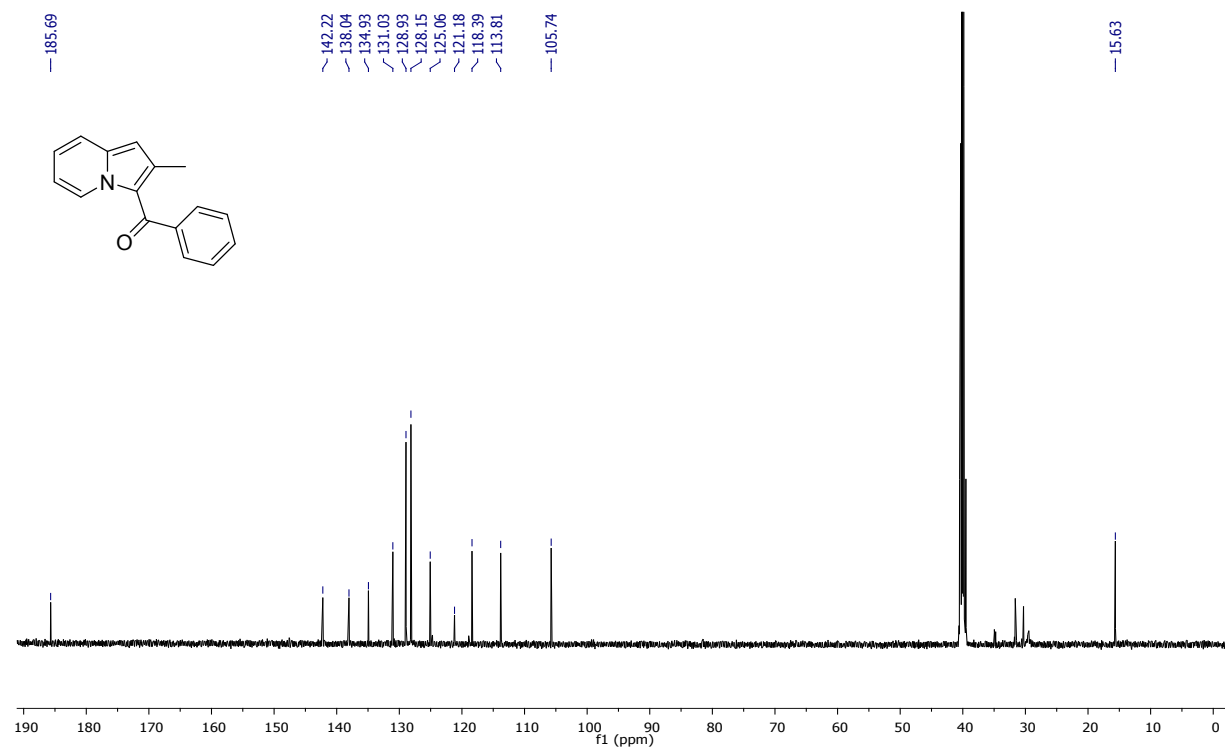
^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) spectrum of **6g**.



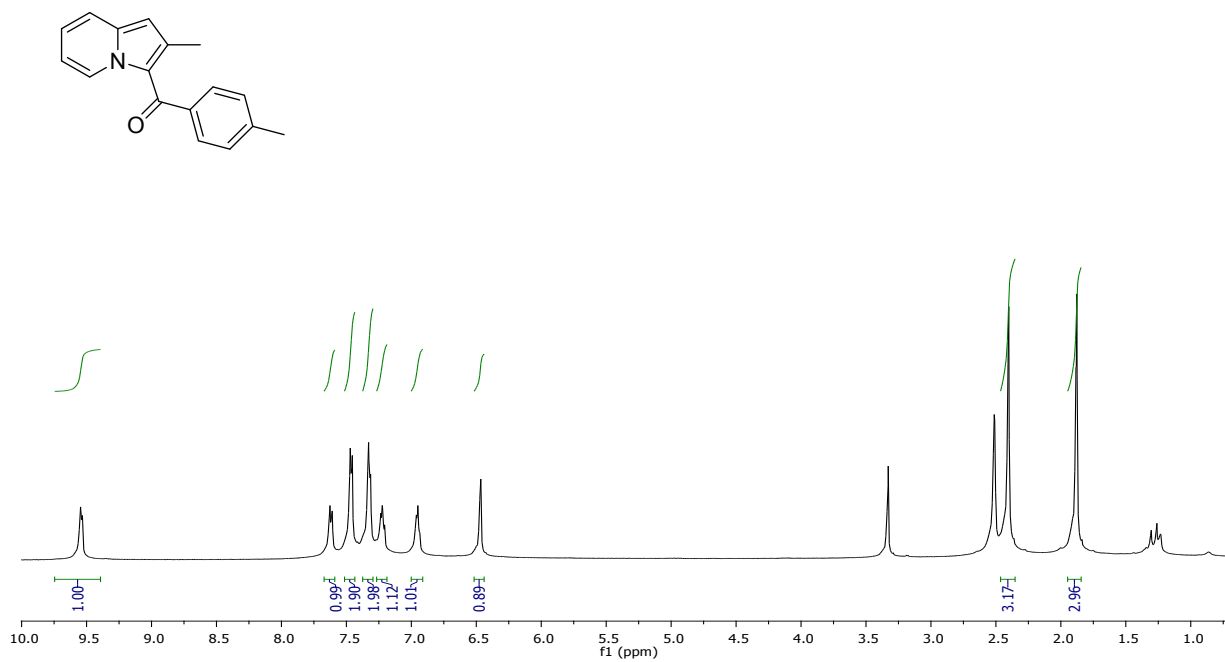
¹H NMR (500 MHz, DMSO-*d*₆) spectrum of **6h**.



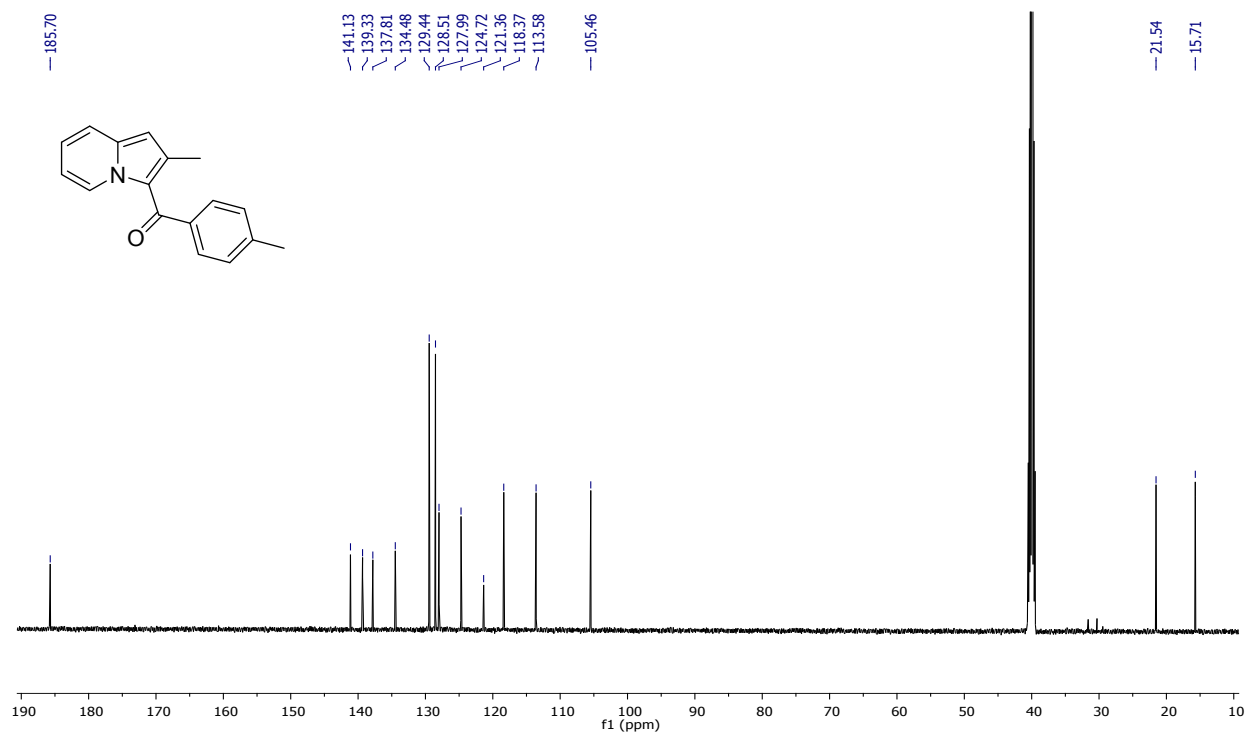
¹H NMR (500 MHz, DMSO-*d*₆) spectrum of **5a'**.



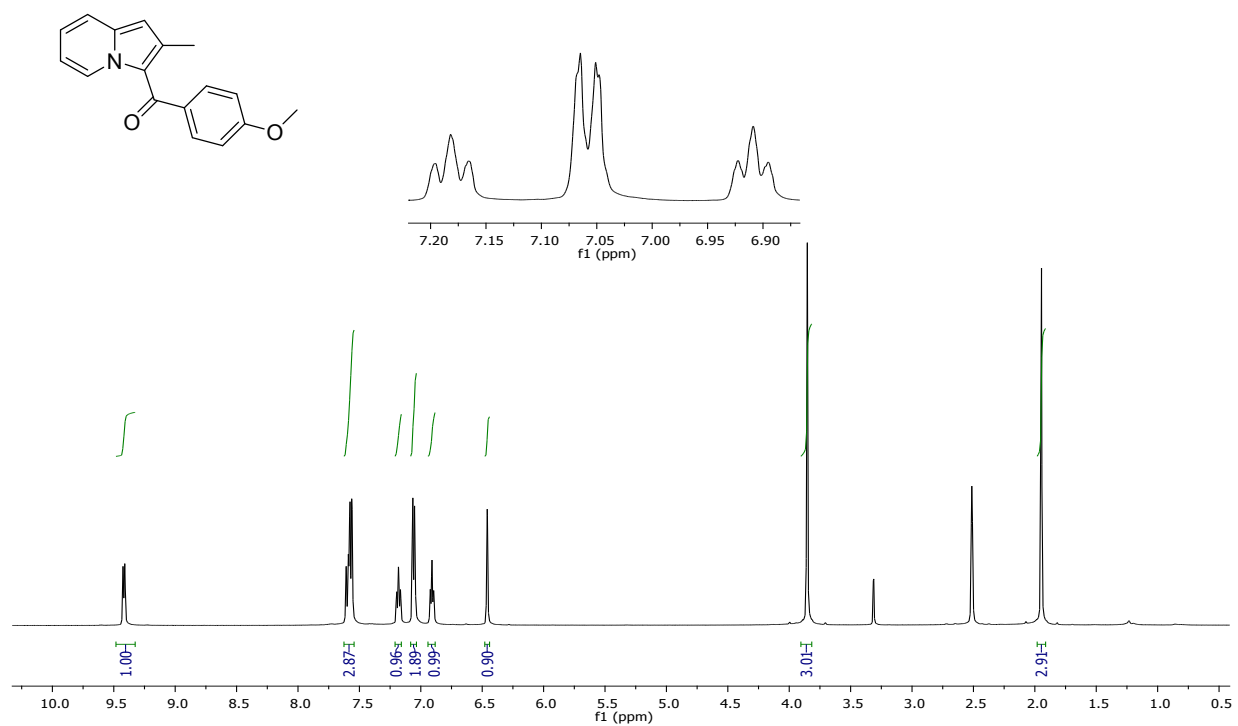
¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of **5a'**.



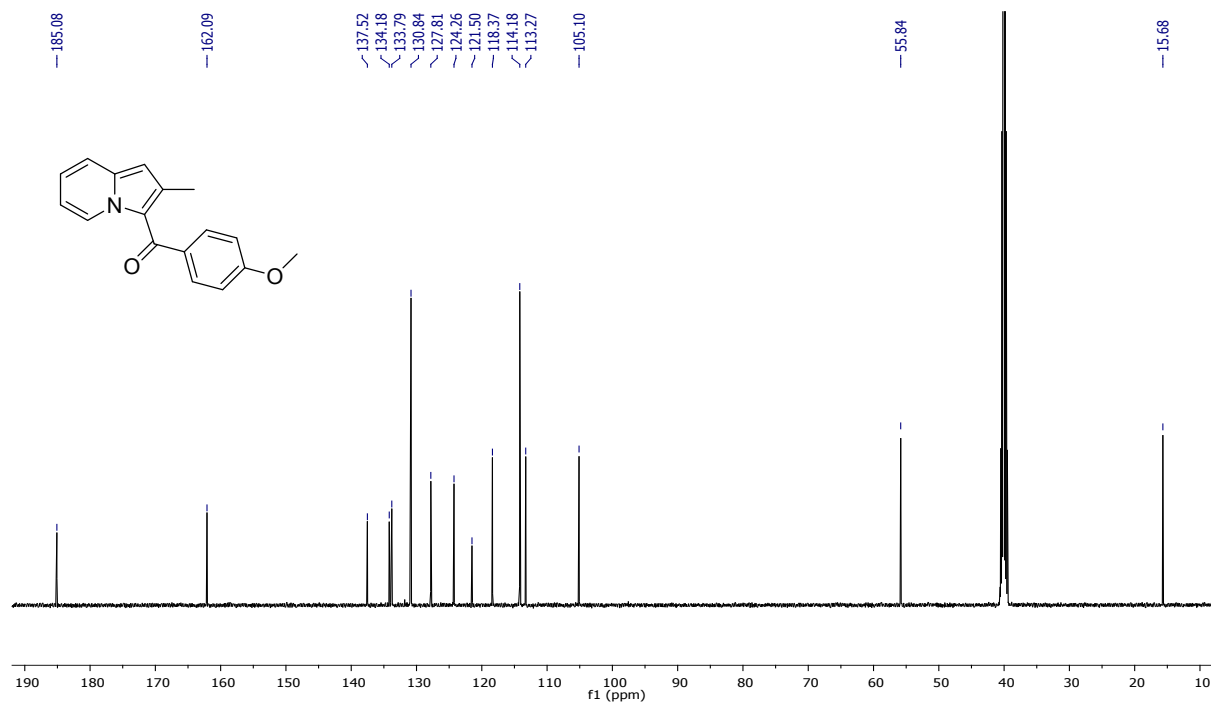
¹H NMR (500 MHz, DMSO-*d*₆) spectrum of **5b'**.



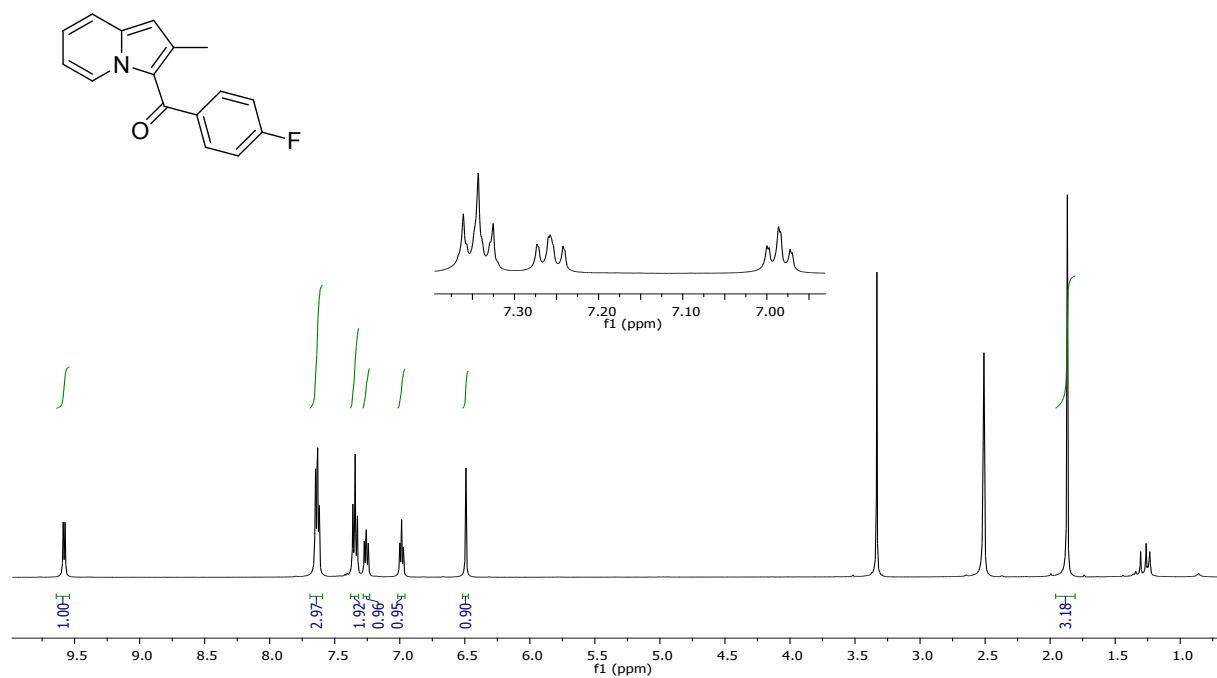
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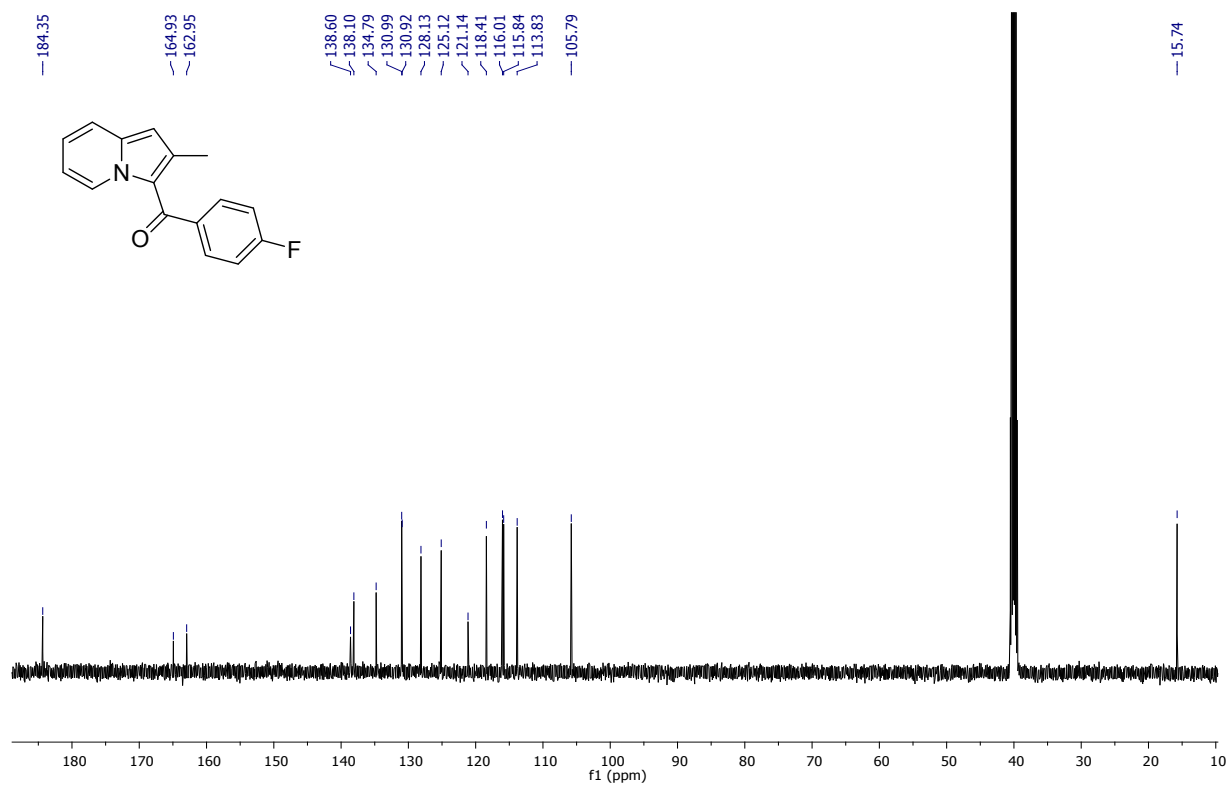
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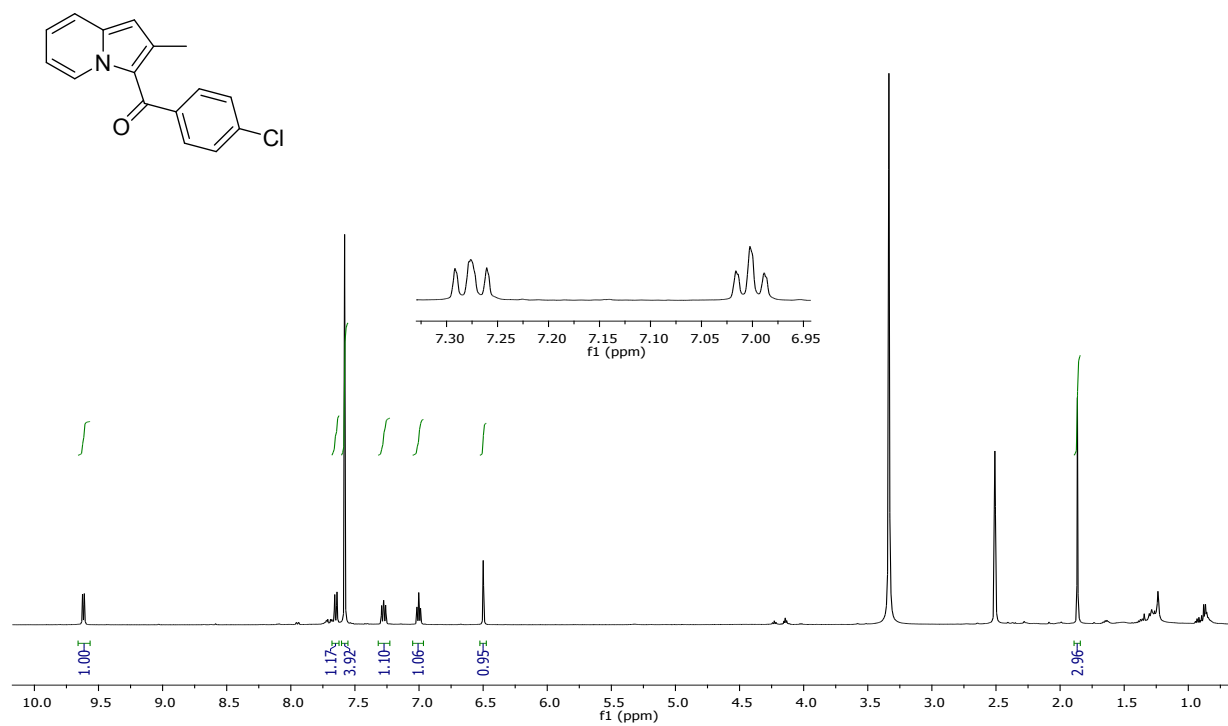
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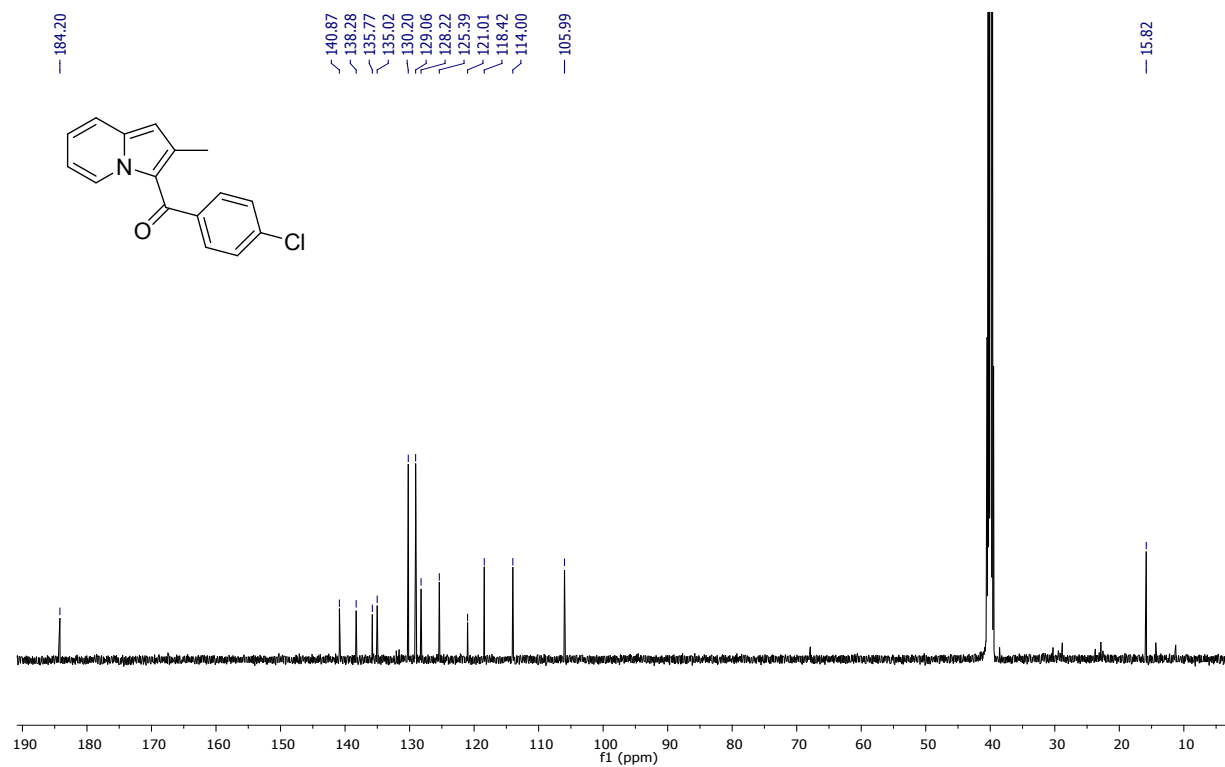
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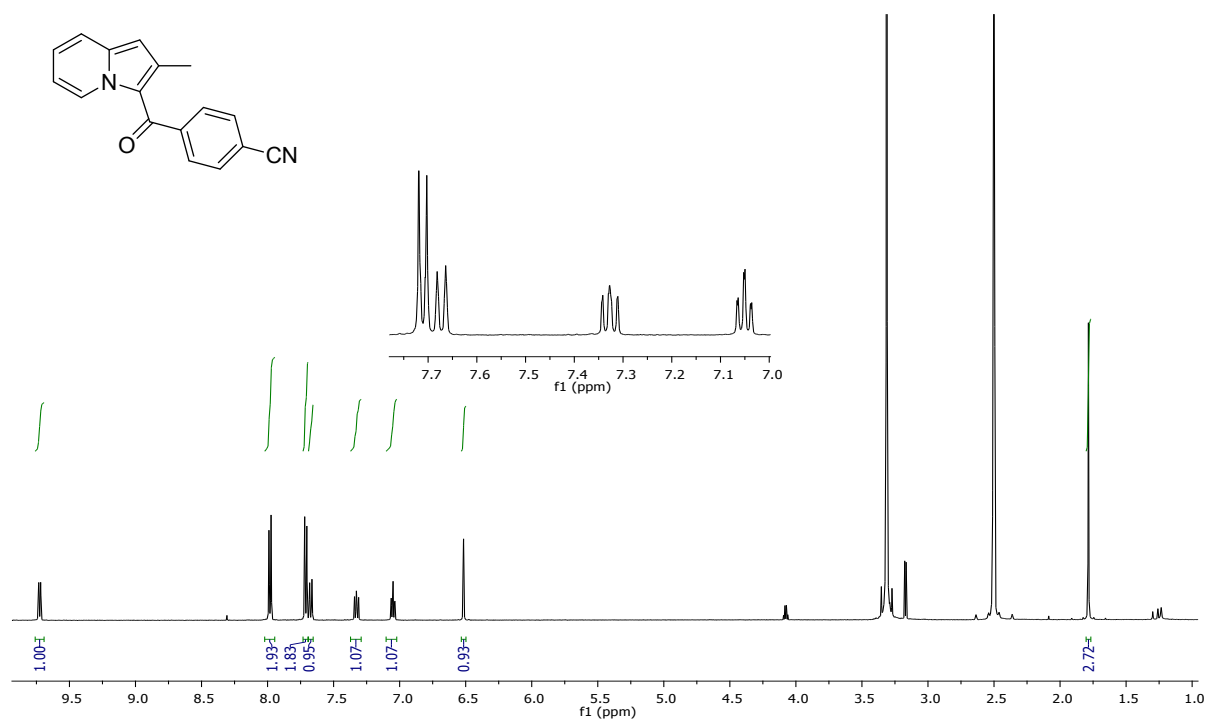
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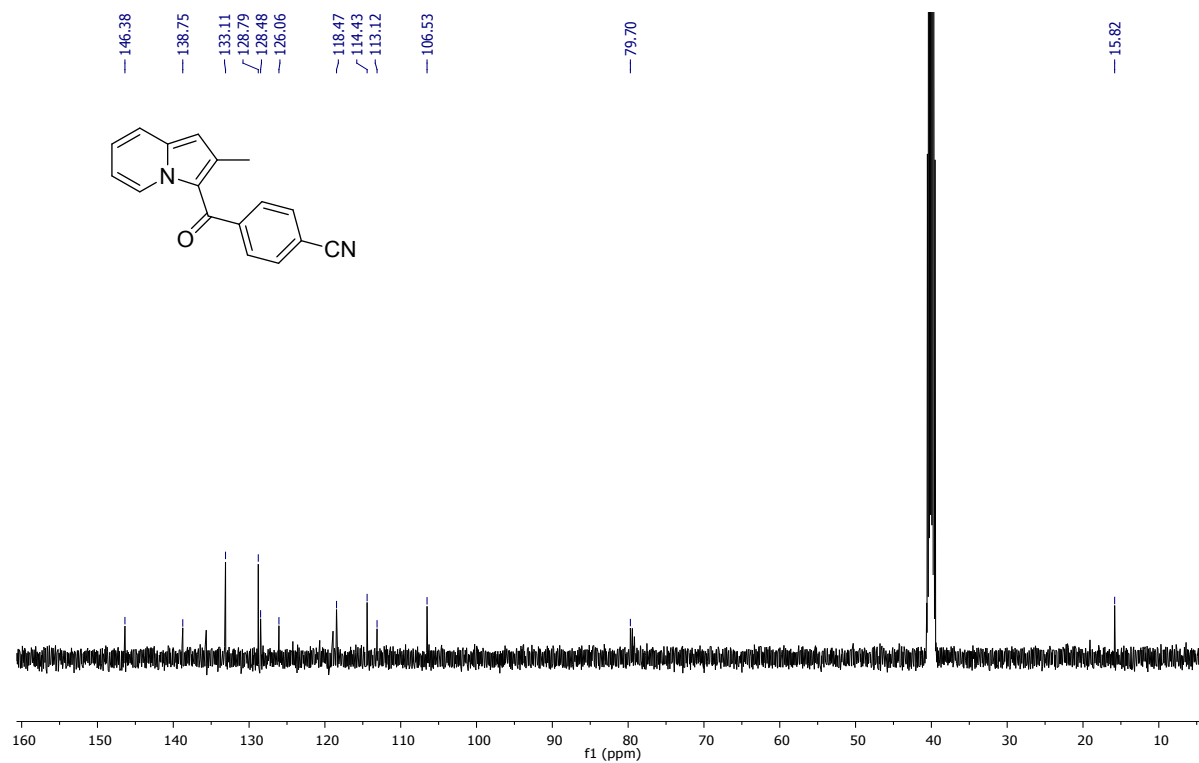
¹H NMR (500 MHz, DMSO-*d*₆) spectrum of **5e'**.



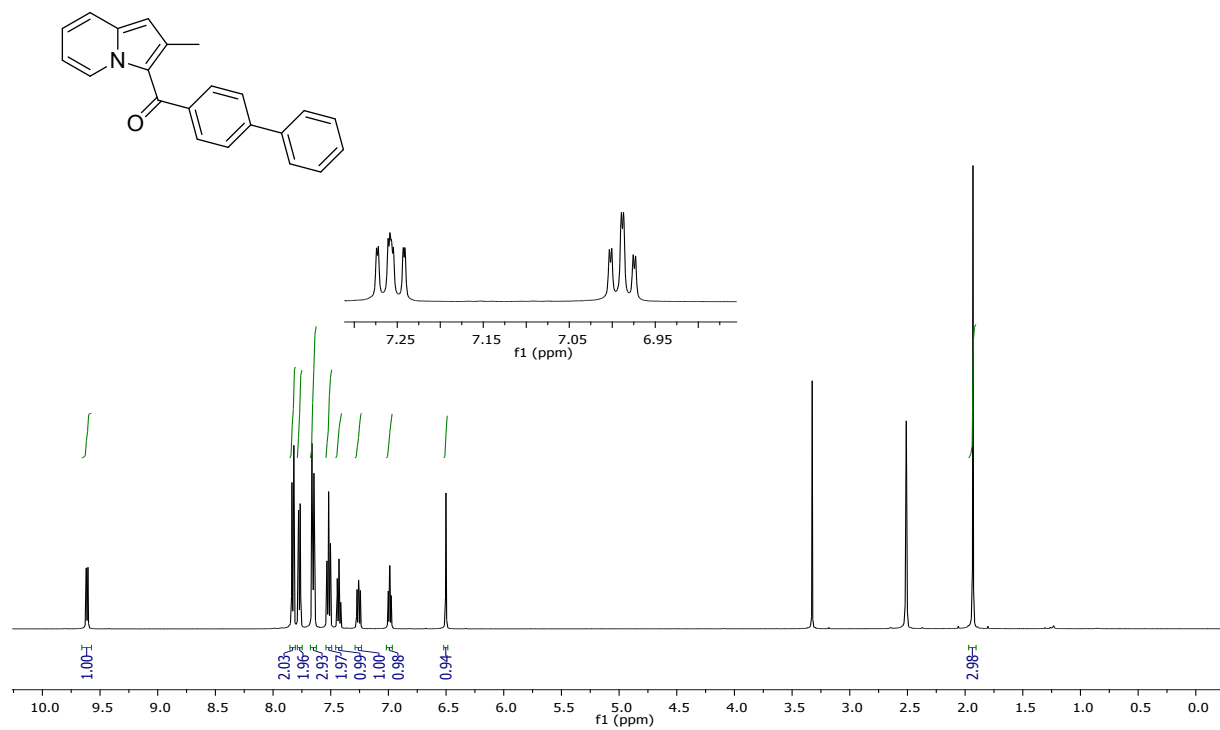
^{13}C NMR (125 MHz, DMSO- d_6) spectrum of **5e**.



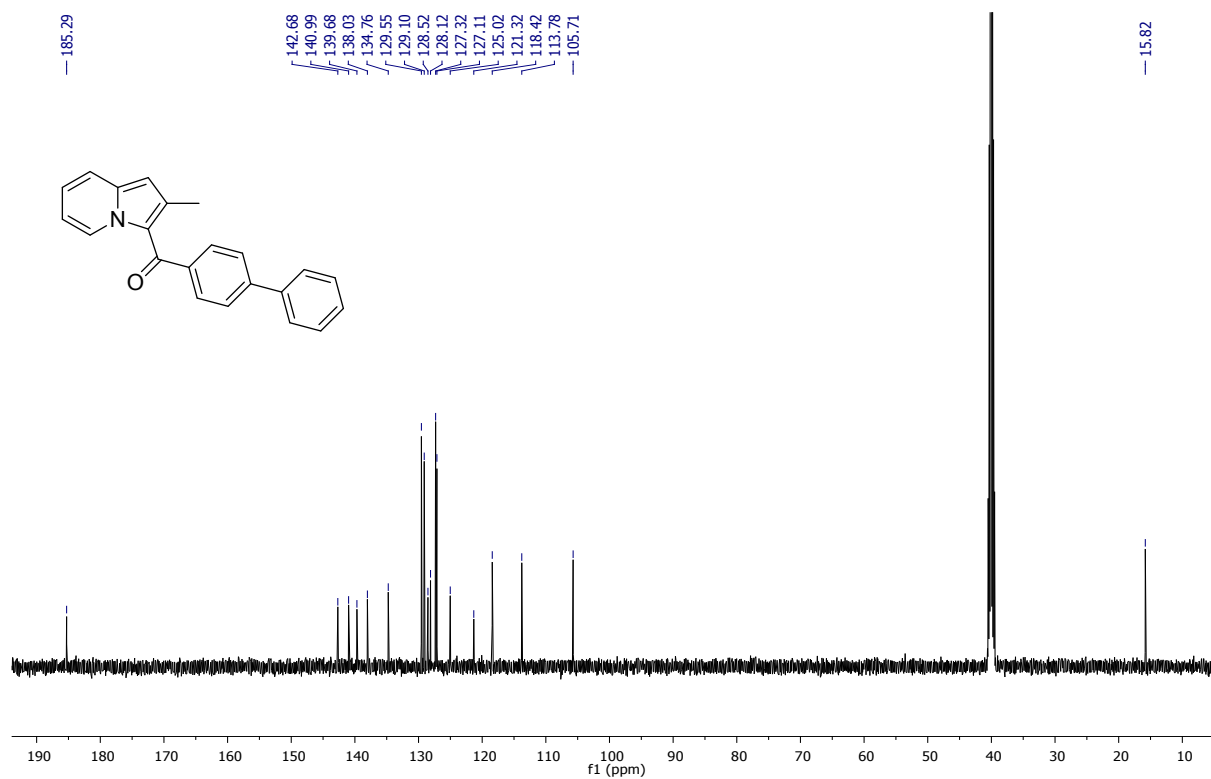
^1H NMR (500 MHz, DMSO- d_6) spectrum of **5f**.



¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of **5f**.



¹H NMR (500 MHz, DMSO-*d*₆) spectrum of **5g**.



¹³C N MR (125 MHz, DMSO-*d*₆) spectrum of **5g'**.

ESI-MS Data

OSPC, Dr RATHOD

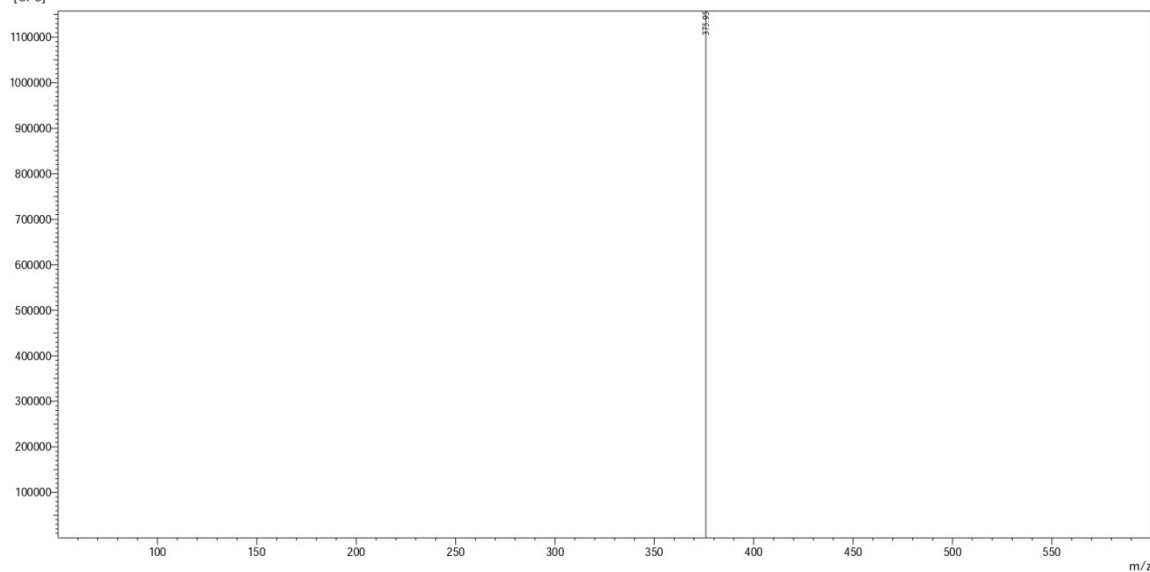
SHIMADZU
LabSolutions

MASS REPORT

Sample Name : A2-347-375
Data File : 25092020.60.lcd
Date Acquired : 9/25/2020 1:39:23 PM
Batch File : 25092020.lcb

MS Spectrum
D:\DATA\SEP 2020\25092020.60.lcd

Averaged ESI Positive+
Spectrum Mode: Averaged 0.350-0.868(151-373)
[CPS]



1

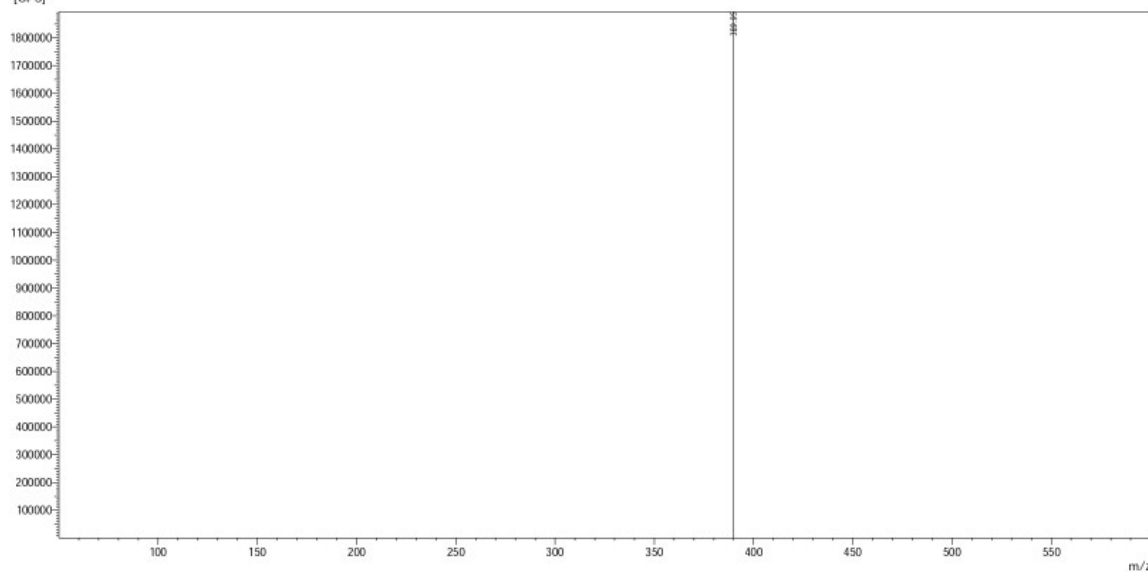
Figure S1a. ESI-MS of 5a.

**MASS REPORT**

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Date Acquired : 9/25/2020 1:41:59 PM
Batch File : 25092020.lcb

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Averaged ESI Positive+
Spectrum Mode: Averaged 0.448-0.770(193-331)
[CPS]



1

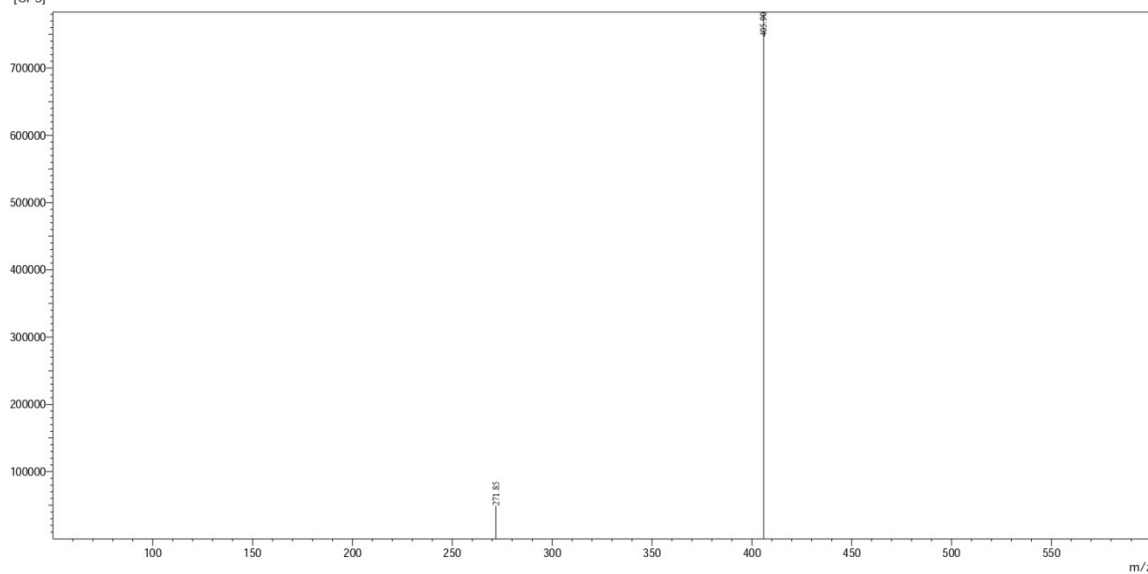
Figure S1b. ESI-MS of 5b.

**MASS REPORT**

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Date Acquired : 9/25/2020 1:44:40 PM
Batch File : 25092020.lcb

MS Spectrum
D:\DATA\SEP 2020\25092020.62.lcd

Averaged ESI Positive+
Spectrum Mode: Averaged 0.411-0.845 (177-363)
[CPS]



1

Figure S1c. ESI-MS of 5c.

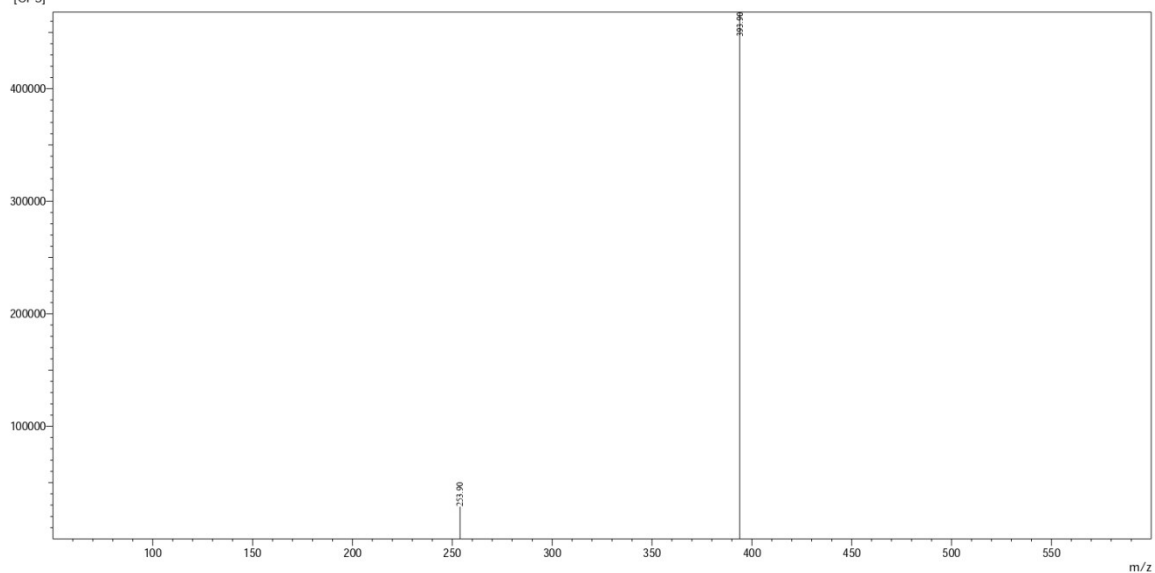


MASS REPORT

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Date Acquired : 9/25/2020 1:15:50 PM
Batch File : 25092020.lcb

MS Spectrum
D:\DATA\SEP 2020\25092020.51.lcd

Averaged ESI Positive+
Spectrum Mode: Averaged 0.401-0.924 (173-397)
[CPS]



1

Figure S1d. ESI-MS of **5d**.

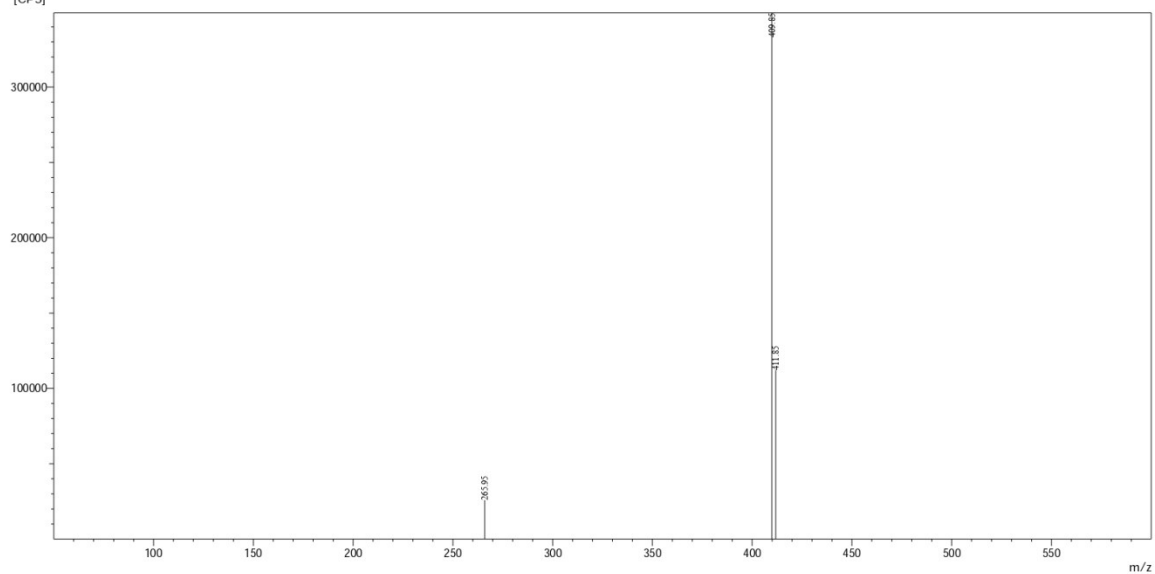


MASS REPORT

Sample Name : B5-409
 Data File : 25092020.55.lcd
 Date Acquired : 9/25/2020 1:26:16 PM
 Batch File : 25092020.lcb

MS Spectrum
 D:\DATA\SEP 2020\25092020.55.lcd

Averaged ESI Positive+
 Spectrum Mode: Averaged 0.341-0.933(147-401)
 [CPS]



1

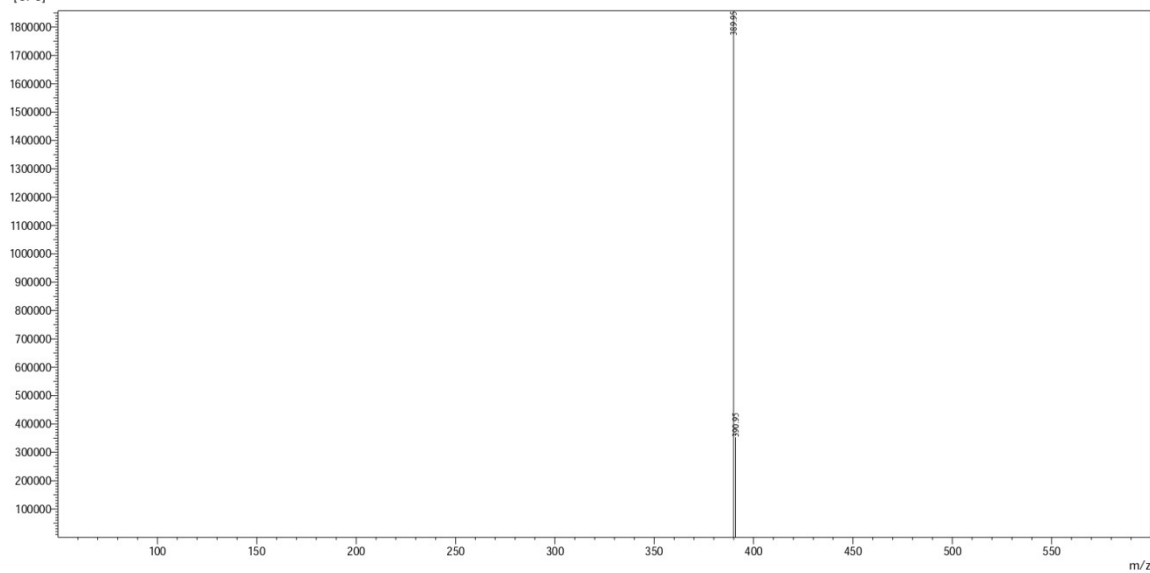
Figure S1e. ESI-MS of 5e.

**MASS REPORT**

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Date Acquired : 9/24/2020 4:10:29 PM
Batch File : 24092020.1cb

MS Spectrum
D:\DATA\SEP 2020\24092020.18.lcd

Averaged ESI Positive+
Spectrum Mode: Averaged 0.429-0.779 (185-335)
[CPS]



1

Figure S1f. ESI-MS of 6a.

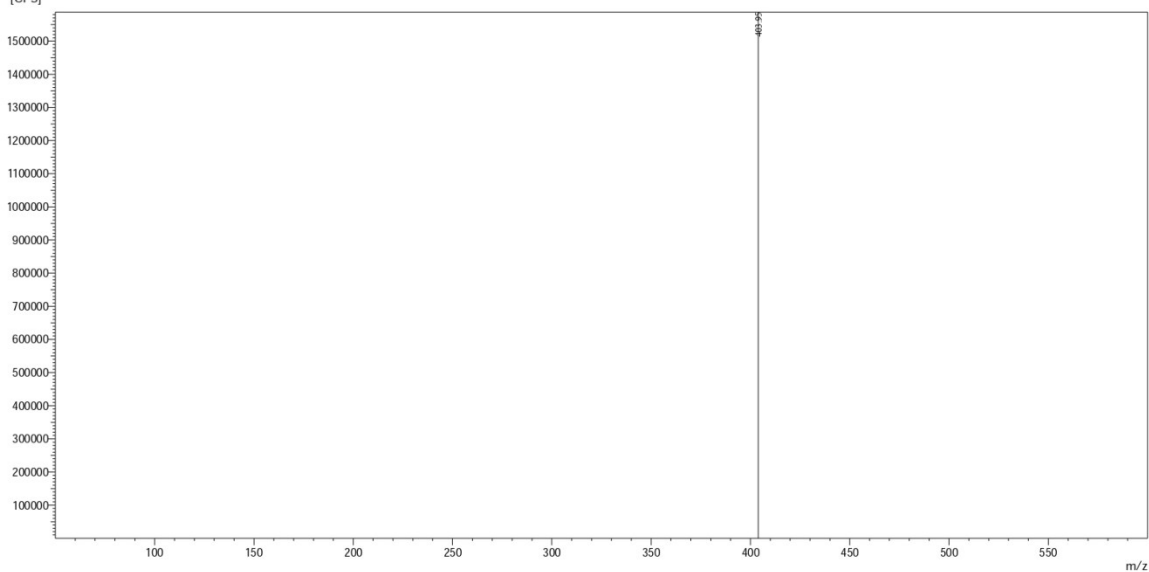


MASS REPORT

Sample Name : A6-351-403
 Data File : 24092020.17.lcd
 Date Acquired : 9/24/2020 4:07:54 PM
 Batch File : 24092020.1cb

MS Spectrum
 D:\DATA\SEP 2020\24092020.17.lcd

Averaged ESI Positive+
 Spectrum Mode: Averaged 0.383-0.779 (165-335)
 [CPS]



1

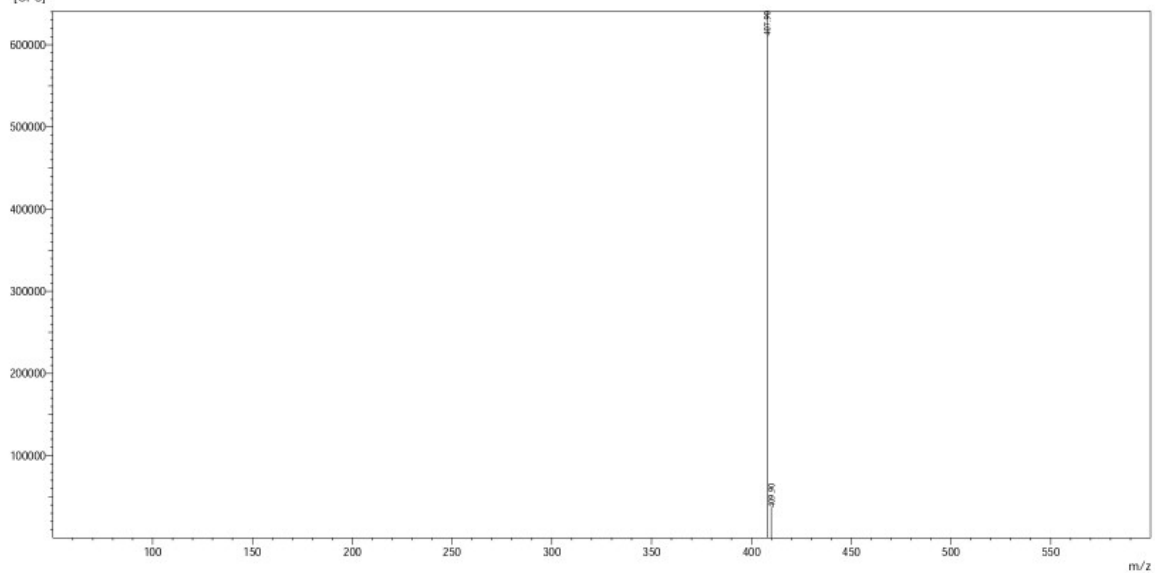
Figure S1g. ESI-MS of 6b.

**MASS REPORT**

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Date Acquired : 9/25/2020 1:34:08 PM
Batch File : 25092020.1cb

MS Spectrum
D:\DATA\SEP 2020\25092020.58.lcd

Averaged ESI Positive+
Spectrum Mode: Averaged 0.364-0.840 (157-361)
[CPS]



1

Figure S1h. ESI-MS of 6d.

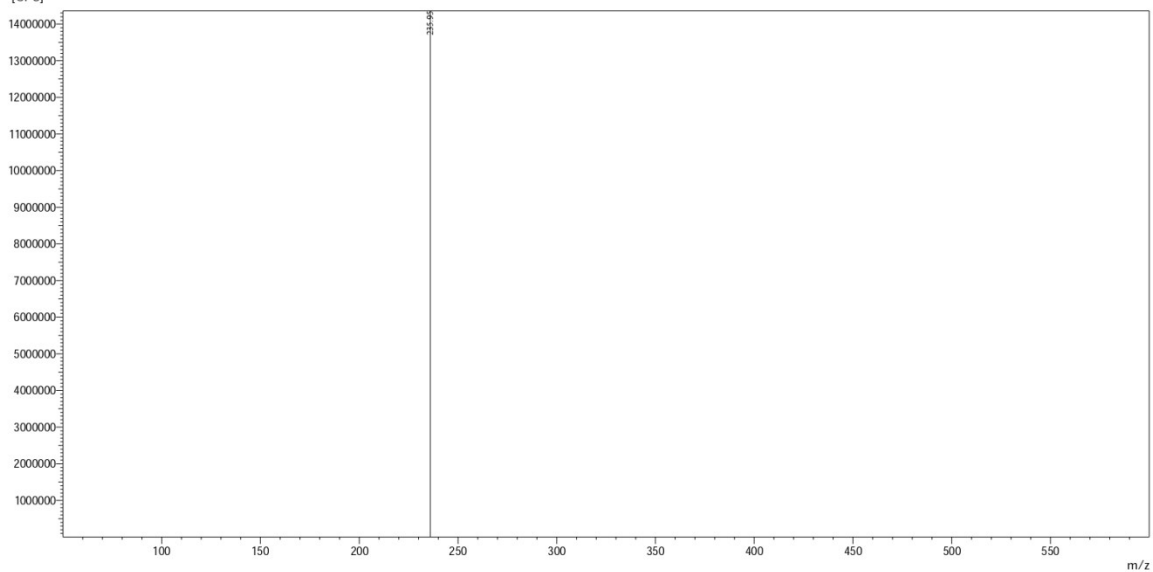


MASS REPORT

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 Date Acquired : 9/25/2020 1:36:44 PM
 Batch File : 25092020.lcb

MS Spectrum
 D:\DATA\SEP 2020\25092020.59.lcd

Averaged ESI Positive+
 Spectrum Mode: Averaged 0.434-0.747 (187-321)
 [CPS]



1

Figure S1i. ESI-MS of 5a'.

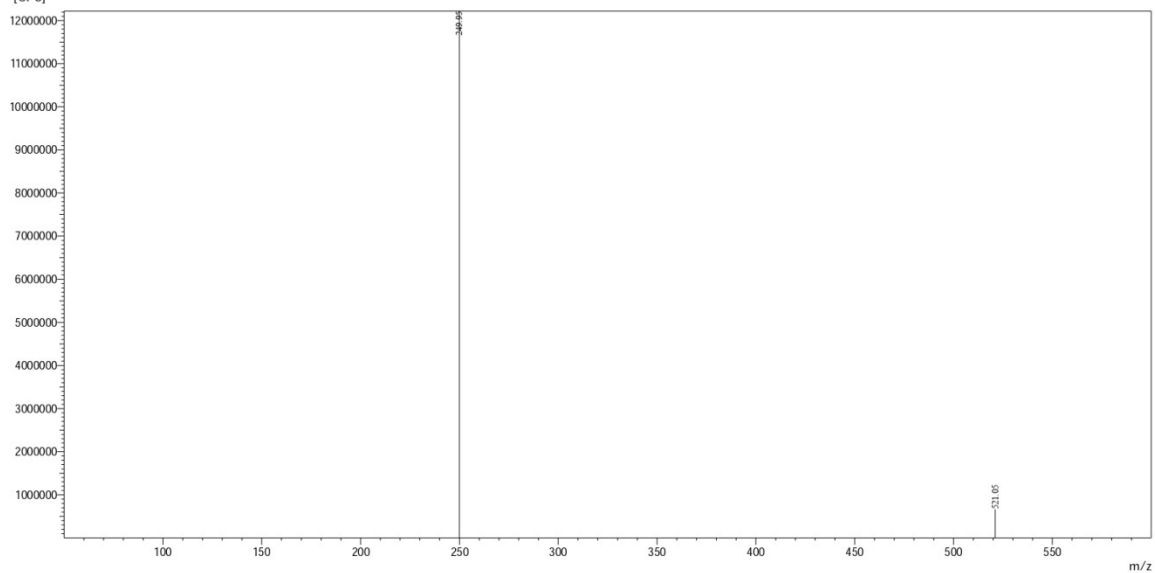


MASS REPORT

Sample Name : A4-349-249
Data File : 24092020.16.lcd
Date Acquired : 9/24/2020 4:05:13 PM
Batch File : 24092020.1cb

MS Spectrum
D:\DATA\SEP 2020\24092020.16.lcd

Averaged ESI Positive+
Spectrum Mode: Averaged 0.406-0.821(175-353)
[CPS]



1

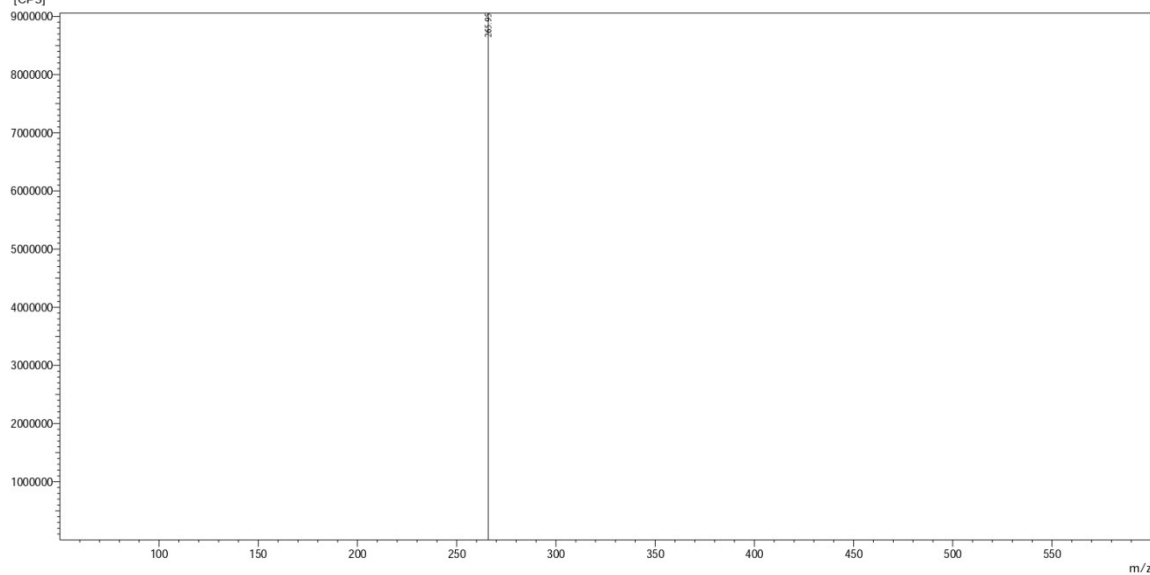
Figure S1j. ESI-MS of 5b'.

**MASS REPORT**

Sample Name : A7-265
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Date Acquired : 9/25/2020 1:21:02 PM
Batch File : 25092020.1cb

MS Spectrum
D:\DATA\SEP 2020\25092020.53.lcd

Averaged ESI Positive+
Spectrum Mode: Averaged 0.401-0.751 (173-323)
[CPS]



1

Figure S1k. ESI-MS of **5c'**.

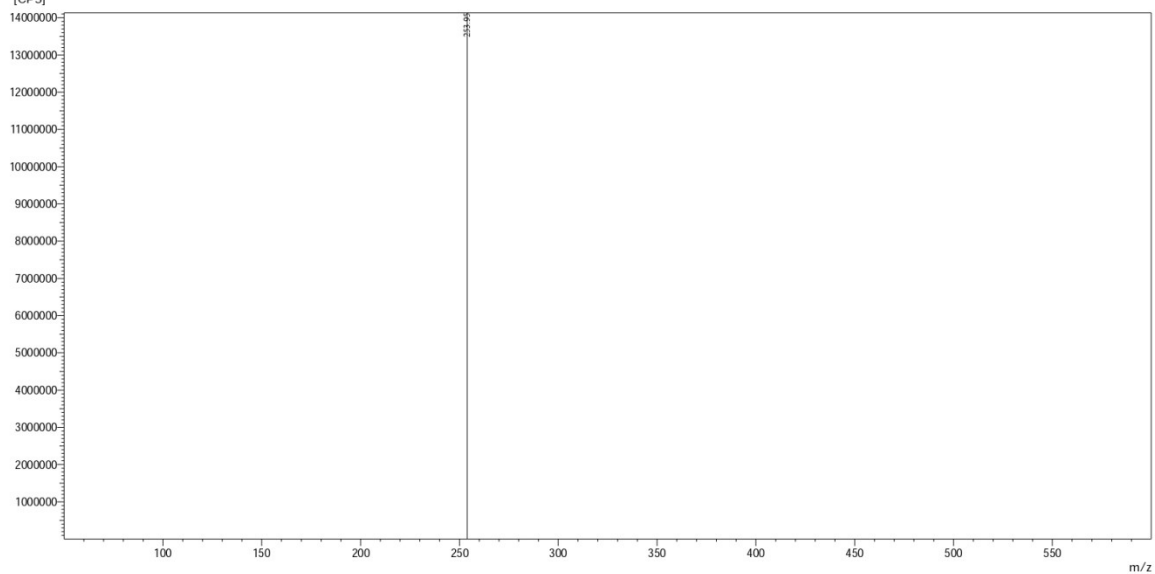


MASS REPORT

Sample Name : A10-355-253
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 Date Acquired : 9/25/2020 1:13:14 PM
 Batch File : 25092020.lcb

MS Spectrum
 D:\DATA\SEP 2020\25092020.50.lcd

Averaged ESI Positive+
 Spectrum Mode: Averaged 0.462-0.747(199-321)
 [CPS]



1

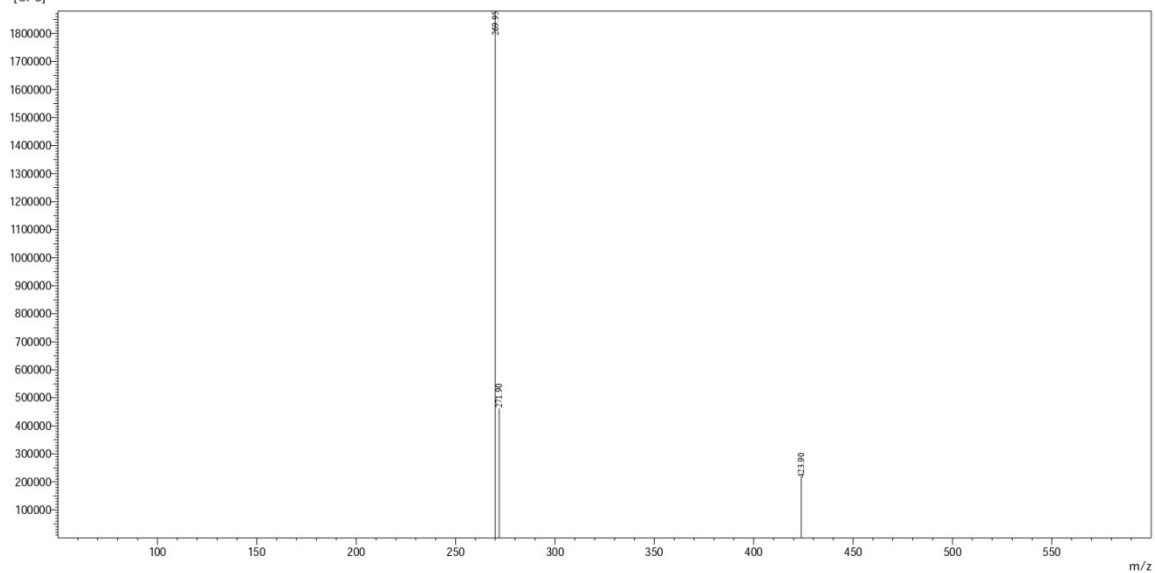
Figure S11. ESI-MS of 5d'.

**MASS REPORT**

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Date Acquired : 9/25/2020 1:23:39 PM
Batch File : 25092020.lcb

MS Spectrum
D:\DATA\SEP 2020\25092020.54.lcd

Averaged ESI Positive+
Spectrum Mode: Averaged 0.387-0.817 (167-351)
[CPS]



1

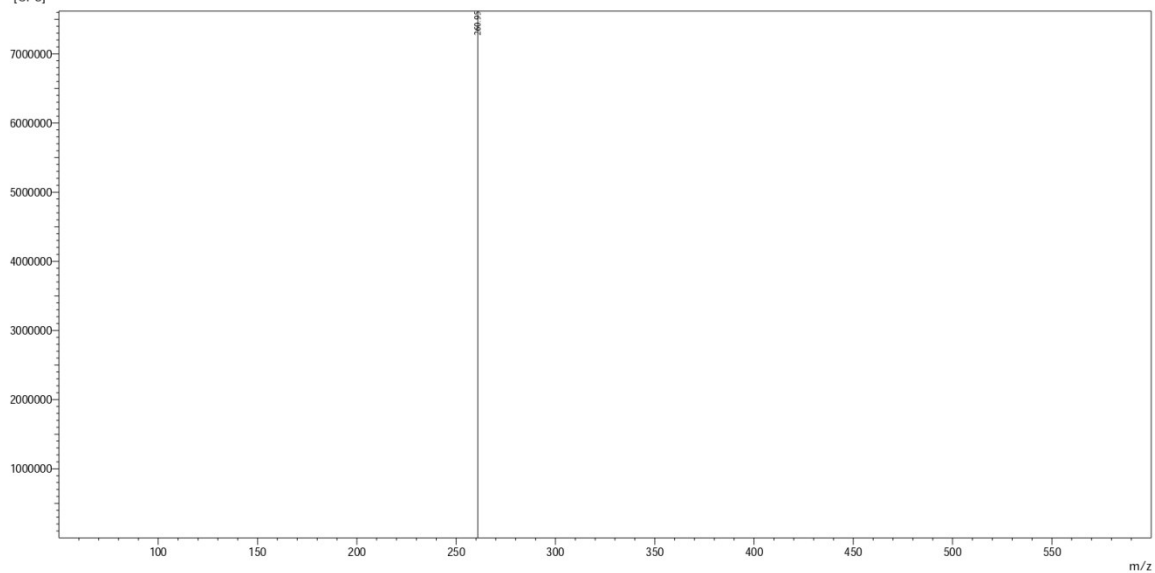
Figure S1m. ESI-MS of 5e'.

**MASS REPORT**

Sample Name : DN-CN-260
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Date Acquired : 9/24/2020 4:02:33 PM
Batch File : 24092020.1cb

MS Spectrum
D:\DATA\SEP 2020\24092020.15.lcd

Averaged ESI Positive+
Spectrum Mode: Averaged 0.453-0.770 (195-331)
[CPS]



1

Figure S1n. ESI-MS of 5f².

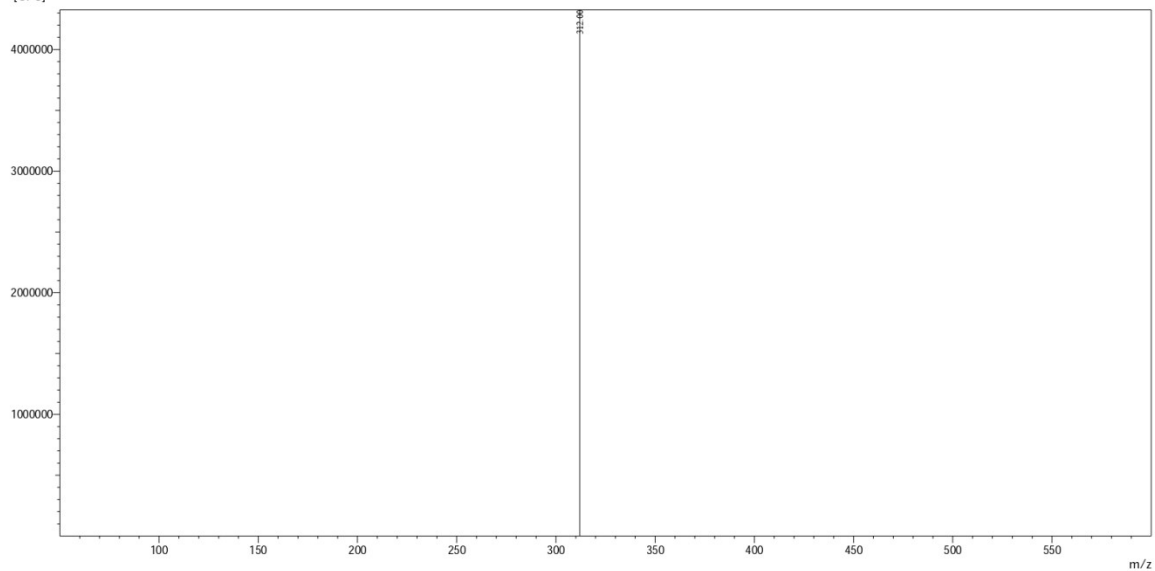


MASS REPORT

Sample Name : DN-503-311
 Data File : 24092020.14.lcd
 Date Acquired : 9/24/2020 3:59:52 PM
 Batch File : 24092020.1cb

MS Spectrum
 D:\DATA\SEP 2020\24092020.14.lcd

Averaged ESI Positive+
 Spectrum Mode: Averaged 0.439-0.919 (189-395)
 [CPS]



1

Figure S1o. ESI-MS of 5g'.